Good Practice Guide

for

Atmospheric Dispersion Modelling

Prepared by the National Institute of Water and Atmospheric Research, Aurora Pacific Limited and Earth Tech Incorporated for the Ministry for the Environment

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Foreword by the Ministry

The introduction of the national environmental standards later this year will see heightened public awareness of air quality issues. Driven largely by a strong need for action on ambient levels of particles in most parts of the country, the standards lay the foundation for an effective air quality management framework. Atmospheric dispersion modelling is an essential tool in air quality management by providing the link between environmental effects and discharges to air. Its use has grown rapidly in New Zealand over the past 10 years and models are now commonplace in many resource consent applications for discharge permits.

Dispersion modelling is a complex process and, as with all models, the results are only as useful as the model itself and how it is used. Many different approaches to modelling have emerged in New Zealand under the Resource Management Act 1991, and at times models have been used incorrectly, causing problems such as inaccurate data, which can mislead an assessment of environmental effects. These issues often delay the processing of resource consents, and can result in expensive hearings where experts argue over the merits of their preferred models and how they should be used.

In a first step to resolving such issues, this draft guide provides expert and well-debated guidance on dispersion modelling through a series of recommended protocols. To improve consistency and accuracy in modelling, the guide is reasonably prescriptive, but the recommendations are not regulatory requirements so there is flexibility to handle the wide variety of circumstances that occur in New Zealand. Deviations from the recommended approaches can be taken, although these should be clearly explained and justified.

Correct interpretation of modelling results against the national environmental standards and determination of the potential effects of a discharge are as important as accurate modelling results. This guide does not include guidance on interpreting results. Instead, this will be included in a *Good Practice Guide for Assessing Discharges to Air* (currently under development by the Ministry).

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Executive Summary

The purpose of this guide is to provide good-practice protocols for modelling the dispersion of discharges to air from industrial complexes in New Zealand. Guidance is provided for all modellers, from relative newcomers to experts. The guideline provides recommendations which direct modellers towards adopting a best practice approach. The recommendations are somewhat prescriptive, but allow flexibility. They are consistent with current practice in Australia and the USA, with some adaptation for New Zealand-specific conditions. The practitioner should always justify the methods used, whichever modelling approach is taken.

For convenience, dispersion model types are divided broadly into steady-state Gaussian-plume models and 'advanced' models. This is a differentiation on roughly historical grounds: plume models have been in common use for decades, while advanced models are beginning to be used more widely for regulatory applications. From a practical standpoint, the greatest difference between model types is in the requirements of meteorological information and computer resources. However, some 'steady-state' models are highly sophisticated and not necessarily 'Gaussian', so the distinction can be blurred. Although the guide encourages modellers to move towards advanced models – because in principle they are more realistic – it does discuss the advantages and limitations of *all* model types. The use of an 'advanced' model need not be the best option.

This guide provides useful guidance for the modeller by discussing specific models currently in use in New Zealand. The list includes AUSPLUME, ISCST3, AERMOD, CTDMPLUS, CALPUFF and TAPM. Model configuration, data requirements, model applicability, physical and chemical formulations and the interpretation of results are discussed for these models.

Much of the guide is devoted to practical advice and provides recommendations on the aspects of dispersion modelling essential to a realistic assessment using a dispersion model. These aspects are the choice of input parameters, the specification of emissions and meteorology, and the analysis of results.

A chapter on model configuration discusses model domain size and receptor distribution, dispersion parameters, stability class specification, the use of turbulence measurements, settings for plume rise and inversion penetration, land-use variations and averaging times. It also describes how the different models simulate emissions from different source types, and provides guidance on emission factor databases and on accounting for time-varying emissions. It further describes how the models simulate the interaction between pollutant plumes from different sources within an industrial complex, in terms of building wake effects and enhanced plume buoyancy.

The simulation of terrain effects on pollutant dispersion is examined in detail, including a description of methods used by the main models.

There is some discussion on atmospheric chemistry – a common requirement is the determination of NO_2 concentrations, given emissions of NO_x. A couple of empirical methods for this are described, although the guide does not favour one over the other.

A complete chapter of this guide is devoted to the meteorological aspects of dispersion modelling. The complex terrain of New Zealand, and the coastal location of most settlements, can lead to highly complicated meteorological features in the vicinity of many pollutant sources. These include land–sea breezes, slope–valley flows and internal boundary layers (with associated fumigation effects), which may cause complex patterns of pollution dispersion.

A fundamental difference between steady-state and advanced models is in their meteorological data requirements. The development of single-site meteorological data for steady-state dispersion models is discussed, including screening data sets, the treatment of calms, missing data, and the derivation of parameters such as stability class and mixing height. The development of three-dimensional time-dependent meteorological data sets for advanced dispersion models using prognostic and diagnostic models is also discussed in detail. The advantages and limitations of all approaches are examined.

Guidance on the analysis of model results is given, to ensure that results are realistic and credible. This includes model validation, assessment of uncertainties and sensitivity tests. Advice is given on the presentation of statistical summaries, tables, graphs and contour plots at the reporting stage. There is also guidance on the incorporation of background concentrations and the assessment of environmental and health effects.

The good practice guide focuses mainly on discharges from industrial sources, but there is some discussion on other specialised applications, such as airshed modelling, dispersion from roadways, regional and long-range transport, accidental releases, steam effects and visibility. Many of the recommendations regarding industrial discharges apply equally to these other cases.

The guide attempts to be forward thinking by acknowledging that dispersion modelling requirements (that is, new applications) and the models themselves are changing, and by providing guidance on the use of the latest, state-of-the-science dispersion models.

1 Introduction

1.1 Aims and objectives

The purpose of this Guide is to provide good practice protocols for carrying out atmospheric dispersion modelling in New Zealand. Where the recommended protocols are not suitable for the particular modelling exercise, the reasons for deviating from them should be clearly explained. In establishing these good practice protocols, the guide aims to improve the use of models in New Zealand and consequently the accuracy of modelling results so they can be relied upon when considering the potential adverse effects of a discharge to air.

The Guide contains information and recommended protocols on many aspects of modelling including: the main types of model available and when to use them, the nature of input data required, and how to get the most accurate results for the level of assessment required. It is designed to assist those relatively new to modelling who may have taken a course or two, and those involved in reviewing modelling outputs for auditing resource consent applications. The 'recommended protocol' shaded boxes should also be useful for expert modellers who are seeking better consistency in how models are used in New Zealand.

It should be recognised that modelling is a complex process and that some training in the form of workshops or courses is advisable before commencing modelling. This Guide will assist in recalling the training you have received and it sets specific protocols to follow where alternative options are available.

The Guide focuses on how to get accurate data once the decision to model has been made. Guidance on when to model and how to interpret modelling results, in terms of evaluating the potential effects of the discharge on the environment, will be contained in a separate document currently being prepared by the Ministry entitled the *Good Practice Guide for Assessing Discharges to Air*. Although these two areas are integrally linked they have been separated to avoid excessive complexity in one document. However, both guidance documents should be reviewed when assessing a discharge to air using dispersion modelling.

Once the decision to model has been made, the Guide can help practitioners to determine:

- which model is most appropriate for the particular circumstances
- what data to put into the model (including emissions data and meteorological data)
- how to run a model effectively
- pitfalls to watch out for
- how to understand the accuracy of modelling results.

The Guide also discusses the advantages and limitations of:

- current practice associated with using steady-state dispersion models as an assessment tool
- new generation models.

The Guide mainly covers the use of dispersion models to assess the effects of pollutants discharged from point (and multiple point) sources. However, modelling of area and line sources is also briefly considered.

Throughout the Guide modellers are encouraged to:

- use the best available information
- comply with the recommendations made in this document and consider applying the guidance
- create an auditable trail of the work undertaken.

The guidance is not intended to replace the detailed user manuals that accompany each dispersion model and these should still be consulted. In addition it should be recognised that the recommendations do not have any regulatory status and they can be deviated from as required and when justified. Neither is the advice in any way government policy.

1.2 Overview

Here is an outline of the information contained in the Guide.

Section 1 (this section) presents the background information that puts atmospheric dispersion models into a wider context and highlights the issues that should be considered before using them.

Section 2 contains a brief review of the Gaussian-plume and advanced models that are commonly used for regulatory applications.

Section 3 contains a brief review of the more specialised applications of dispersion modelling.

Section 4 details processes for determining information that should go into an atmospheric dispersion model to ensure good quality information is obtained.

Section 5 details the importance of, and methods for, acquiring reliable and representative meteorological input for air quality modelling purposes. The meteorological requirements of advanced dispersion models are described and methods by which these requirements can be met are discussed.

Section 6 describes how to present and explain modelling results clearly and simply, including the interpretation of modelling results and addressing the uncertainty in model predictions.

1.3 What is an atmospheric dispersion model?

A model is a simplified picture of reality. It doesn't contain all the features of the real system but contains the features of interest for the management issue or scientific problem we wish to solve by its use. Models are widely used in science to make predictions and/or to solve problems, and are often used to identify the best solutions for the management of specific environmental problems.

Models may be:

- physical – a scaled-down representation of reality
- mathematical – a description of the system using mathematical relationships and equations.

Contaminants discharged into the air are transported over long distances by large-scale air-flows and dispersed by small-scale air-flows or turbulence, which mix contaminants with clean air. This dispersion by the wind is a very complex process due to the presence of different-sized eddies in atmospheric flow. Even under ideal conditions in a laboratory the dynamics of turbulence and turbulent diffusion are some of the most difficult in fluid mechanics to model. There is no complete theory that describes the relationship between ambient concentrations of air pollutants and the causative meteorological factors and processes.

An atmospheric dispersion model is a:

- mathematical simulation of the physics and chemistry governing the transport, dispersion and transformation of pollutants in the atmosphere
- means of estimating downwind air pollution concentrations given information about the pollutant emissions and nature of the atmosphere.

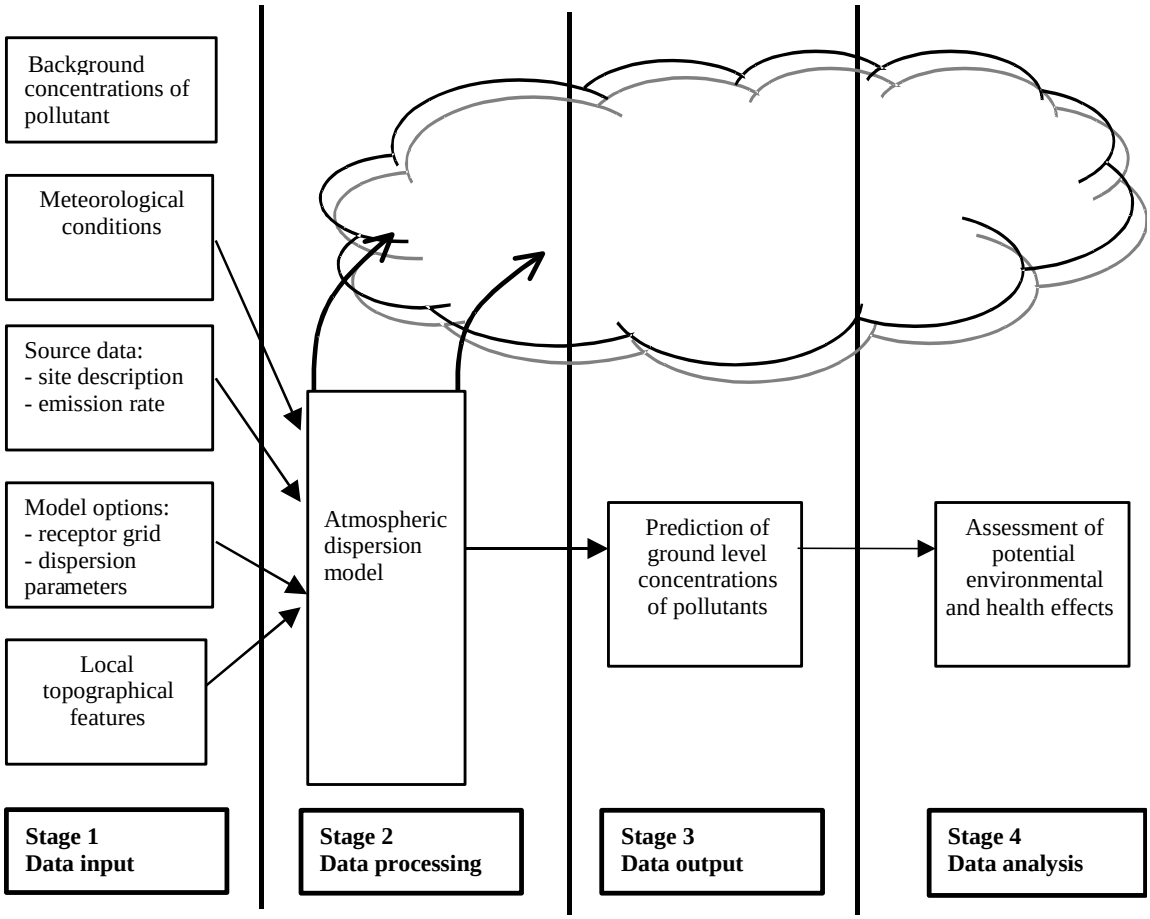
Dispersion models can take many forms. The simplest are provided in the form of graphs, tables or formulae on paper. Today dispersion models more commonly take the form of computer programs, with user-friendly interfaces and online help facilities.

Most modern air pollution models are computer programs that calculate the pollutant concentration downwind of a source using information on the:

- contaminant emission rate
- characteristics of the emission source
- local topography
- meteorology of the area
- ambient or background concentrations of pollutant.

A generic overview of how this information is used in a computer-based air pollution model is shown in Figure 1.1.

Figure 1.1: Overview of the air pollution modelling procedure



The process of air pollution modelling contains four stages (data input, dispersion calculations, deriving concentrations, and analysis). The accuracy and uncertainty of each stage must be known and evaluated to ensure a reliable assessment of the significance of any potential adverse effects.

Currently, the most commonly used dispersion models are steady-state Gaussian-plume models. These are based on mathematical approximation of plume behaviour and are the easiest models to use. They incorporate a simplistic description of the dispersion process, and some fundamental assumptions are made that may not accurately reflect reality. However, even with these limitations, this type of model can provide reasonable results when used appropriately.

More recently, better ways of describing the spatially varying turbulence and diffusion characteristics within the atmosphere have been developed. The *new generation* dispersion models adopt a more sophisticated approach to describing diffusion and dispersion using the fundamental properties of the atmosphere rather than relying on general mathematical approximation. This enables better treatment of difficult situations such as complex terrain and long-distance transport.

Sections 2 and 3 provide detailed descriptions of the different dispersion models available, what each model can potentially be used for, and their benefits and problems.

1.4 The importance of meteorology

The ground-level concentrations resulting from a constant discharge of contaminants change according to the weather (particularly the wind) conditions at the time. Meteorology is fundamental for the dispersion of pollutants because it is the primary factor determining the diluting effect of the atmosphere. Therefore, it is important that meteorology is carefully considered when modelling.

The importance of, and methods for, acquiring reliable and representative meteorological input for air quality modelling purposes are detailed in section 5.

1.5 What can dispersion modelling be used for?

Models can be set up to estimate downwind concentrations of contaminants over varying averaging periods – either short term (three minutes) or long term (annual). In New Zealand, the most common use of dispersion modelling is to assess the potential environmental and health effects of discharges to air from industrial or trade premises. Such assessments are required to be undertaken in accordance with the Resource Management Act 1991 (RMA) for applications for discharge permits. Models are particularly valuable for assessing the impacts of discharges from new activities and to estimate likely changes as a result of process modifications.

Modelling results can also be used for:

- assessing compliance of emissions with air quality guidelines, criteria and standards
- planning new facilities
- determining appropriate stack heights
- managing existing emissions
- designing ambient air monitoring networks
- identifying the main contributors to existing air pollution problems
- evaluating 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 the influence of geophysical factors on dispersion (e.g. terrain elevation, presence of water bodies and land use)
- running ‘numerical laboratories’ for scientific research involving experiments that would otherwise be too costly in the real world (e.g. tracking accidental hazardous substance releases, including foot-and-mouth disease)
- saving cost and time over monitoring – modelling costs are a fraction of monitoring costs and a simulation of annual or multi-year periods may only take a few weeks to assess.

1.6 What can't dispersion models do?

Even the most sophisticated atmospheric dispersion model cannot predict the precise location, magnitude and timing of ground-level concentrations with 100% accuracy. However, most models used today (especially the US EPA approved models) have been through a thorough model evaluation process and the modelling results are reasonably accurate, provided an appropriate model and input data are used.

Errors are introduced into results by the inherent uncertainty associated with the physics and formulation used to model dispersion, and by imprecise input parameters, such as emission and meteorological data. The most significant factors that determine the quality and accuracy of the results are:

- the suitability of the model for the task
- the availability of accurate source information
- the availability of accurate meteorological data.

The causes of model uncertainty and the methods by which they should be addressed when using dispersion models are discussed in more detail in section 6.2.

1.7 When is it appropriate to use dispersion modelling as an assessment tool?

Atmospheric dispersion models may not always be the most appropriate method for assessing the potential environmental impacts of a discharge to air. Guidance on when modelling is required as part of an assessment of environmental effects will be covered in more detail in the *Good Practice Guide for Assessing Discharges to Air* currently under development by the Ministry.

Modelling is unlikely to be needed when a discharge is already permitted by a regional plan. However, councils may specify when modelling is required for particular activities. Assessors should consult with relevant councils to determine whether modelling is required before commencing assessments and submitting applications.

Recommendation 1

Before undertaking an assessment of effects using atmospheric dispersion modelling, the proposed approach for assessing adverse effects should be discussed with the relevant council (national guidance will be covered in the *Good Practice Guide for Assessing Discharges to Air* currently under development by the Ministry).

Alternative and perhaps more pragmatic methods of providing information to support assessments should be employed when the scale of the activity is small and its potential environmental effects are likely to be minor, or when modelling is unlikely to provide good-quality information.

Atmospheric dispersion models should only be used when they are appropriate for investigating the scale and significance of the effects of a discharge on the environment, and their use should be justified.

Users must recognise that there are limitations to the scope of a model's application and to the accuracy of model predictions. These should be identified and discussed in conjunction with the modelling results.

Modelling results provide reasonably accurate predictions of ground-level concentrations of contaminants from a discharge, provided input parameters are appropriate. Factors influencing their accuracy should be estimated, reported and acknowledged.

2 Which Dispersion Model To Use?

One of the key elements of an effective dispersion modelling study is to choose an appropriate tool to match the scale of impact and complexity of a particular discharge. When choosing the most appropriate model the principal issues to consider are:

- the complexity of dispersion (e.g. terrain and meteorology effects)
- the potential scale and significance of potential effects, including the sensitivity of the receiving environment (e.g. human health versus amenity effects).

For regulatory purposes in New Zealand, there are two general types of dispersion models that can be used:

- Gaussian-plume models such as AUSPLUME, ISCST3 (EPA[1]), AERMOD (EPA[2]) and CTDMPLUS (Perry et al., 1989)
- advanced models such as CALPUFF (Scire et al., 2000a) and The Air Pollution Model (TAPM) (Hurley, 2002).

Figure 2.1 illustrates the types of models typically applied to particular scenarios, depending on their scale and complexity. The width of the band associated with each model type is roughly proportional to the number of modellers currently using that particular type. In medium-complex atmospheric and topographical conditions with relatively simple effects, Gaussian-plume models can produce reliable results. This modelling accounts for the vast majority of dispersion modelling work in New Zealand. In more complex atmospheric and topographical conditions, advanced puff or particle models and meteorological modelling may be required to maintain a similar degree of accuracy. In choosing the most appropriate model it is very important to understand the model's limitations and apply it only to the situations that match its capabilities.

The choice of an appropriate dispersion model is heavily dependent on the intended application. Many of New Zealand's major cities are located within 20 kilometres of the coast and so the majority of air pollution concentrations over urban areas are affected by highly variable coastal airflows. The situation is further complicated by complex topography. In such environments simple Gaussian-plume models may not provide the best results. This is likely to be especially true if pollutants cause effects at distances greater than about 10 kilometres from their source and under fumigation conditions. In these situations an advanced dispersion model may be more suited to the situation and provide better results.

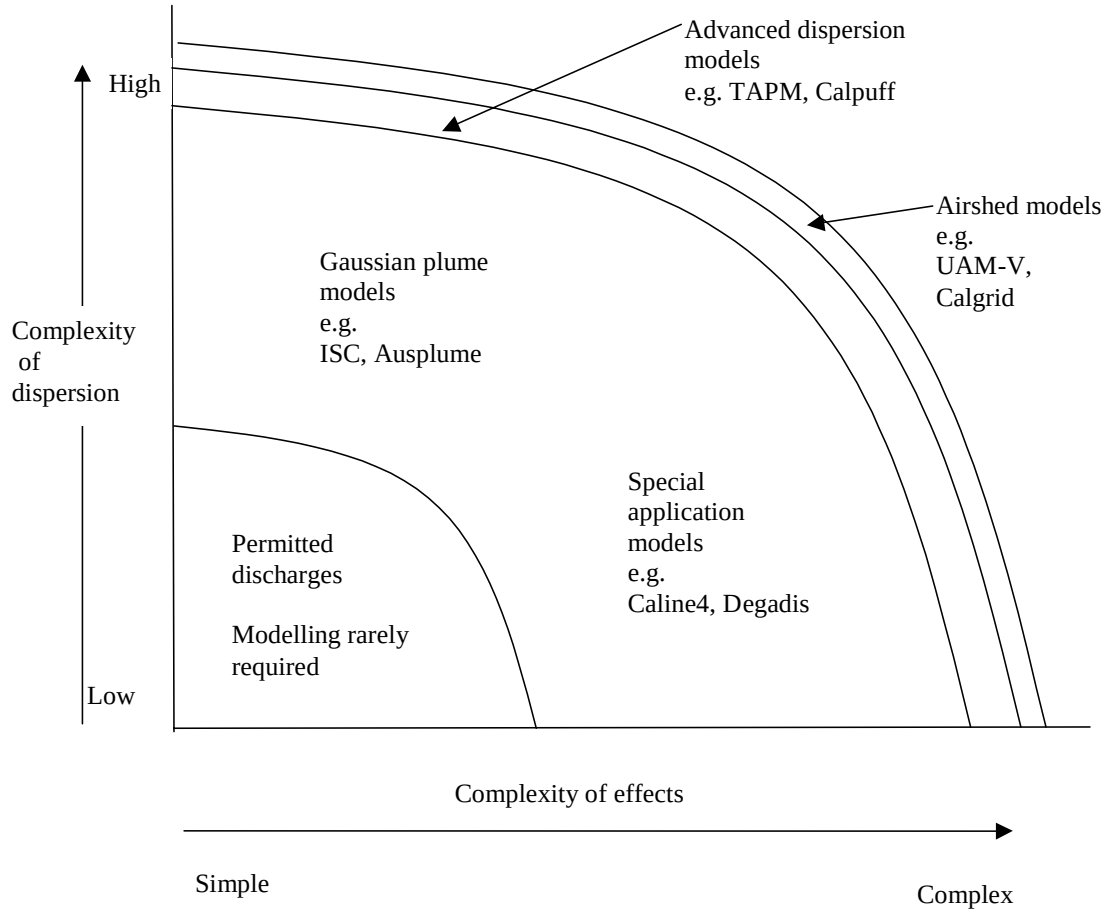
Recommendation 2

To get the best possible results from a dispersion modelling study, the modeller must:

a) choose the most appropriate model for the intended purpose, and

b) justify this choice in the methodology of the study.

Figure 2.1: Type of model typically applied according to the complexity of the problem



In situations of complex terrain or near coastal boundaries, significant changes in meteorological conditions can occur over short distances. Advanced models can simulate the effects of coastal areas and terrain effects on pollutant transport and dispersion in a much more realistic way than a Gaussian-plume model, which assumes spatial uniformity in the meteorology. Clearly this means that advanced models require more detailed meteorological input data to accurately emulate the complex dispersion effects.

Some advanced models are seldom used in regulatory applications due to their complexity, long run-times and inability to model accurately at fine scales. Model developers are attempting to resolve these issues, and advanced models are anticipated to play an increasingly important and more frequent role in the regulatory environment.

Recommendation 3

The following criteria should be used to decide whether to use a Gaussian-plume model or an advanced model.

a) Are you looking at near or far-field impacts?
Plume models are usually only applicable to near-field (within 10 km from the source) calculations. It not wise to assume the meteorology will be the same greater than 10 km away as at the source.

b) Are causality issues important (i.e. the length of time taken for the pollutants to travel from point A to point B)?
Plume models shoot out 'light beams' to infinity and do not take into account the time for the plume to travel from one point to another.

c) Is wet or dry deposition of pollutants likely to be an issue?
There is currently no option to model either wet or dry gas deposition using AERMOD or CTDMPLUS. ISCST3 currently has the same algorithms as CALPUFF for modelling wet and dry deposition of gases and particles. AUSPLUME (5.2) and AERMOD have a crude reflection coefficient algorithm for estimating particle deposition.

d) Do you want to consider SO_x and NO_x chemistry?
The plume models treat SO_x and NO_x chemistry as a simple exponential decay, but do not attempt to address the detailed mechanisms of atmospheric chemistry. Alternatively, they can simulate some chemical processes (e.g. the production of NO_2 from NO_x) as a post-processing step. Advanced models can deal with SO_x, NO_x and organic chemistry, aqueous-phase chemistry and secondary aerosol production.

e) Is your source in a region of complex terrain or a coastal environment?
Meteorology is not uniform in such situations, due to sea breezes or slope and valley flows or other meteorological phenomena. Most Gaussian-plume models do not allow for plume channelling caused by topography. CTDM and ADMS3 are exceptions.

f) Do you suspect inversion break-up fumigation to be an issue?
Most plume models are unable to model inversion-break-up fumigation events. OCD and DISPMOD are exceptions. SCREEN3 can be used for a preliminary assessment of fumigation events.

g) Are stable night-time stagnation events likely to occur?
Gaussian-plume models are unlikely to accurately model stagnation events.

2.1 Gaussian-plume models

Gaussian-plume models are widely used, well understood, easy to apply, and until more recently have received international approval. Even today, from a regulatory point of view ease of application and consistency between applications is important. Also, the assumptions, errors and uncertainties of these models are generally well understood, although they still suffer from misuse.

Gaussian-plume models play a major role in the regulatory arena. However, they may not always be the best models to use and it was noted at the 15th International Clean Air Conference 2000 – Modelling Workshop, that particular models are not always chosen on an objective scientific basis (Ross, 2001).

The Gaussian-plume formula is derived assuming 'steady-state' conditions. That is, the Gaussian-plume dispersion formulae do not depend on time, although they do represent an ensemble time average. The meteorological conditions are assumed to remain constant during the dispersion from source to receptor, which is effectively instantaneous. Emissions and meteorological conditions can vary from hour to hour but the model calculations in each hour are independent of those in other hours. Due to this mathematical derivation, it is common to refer to Gaussian-plume models as steady-state dispersion models. In practice, however, the plume characteristics do change over time, because they depend on changing emissions and meteorological conditions. One consequence of the plume formulation is that each hour the plume extends instantaneously out to infinity. Concentrations may then be found at points too distant for emitted pollutants to have reached them in an hour.

Steady-state models calculate concentrations for each hour from an emission rate and meteorological conditions that are uniform across the modelling domain. Thus they simulate hourly-average concentrations. Both Gaussian-plume and advanced modelling are time-varying, changing from hour to hour. The term 'steady-state' should not be taken to mean that conditions are steady from hour to hour. The plume formula has the uniform wind speed in the denominator and hence breaks down in calm conditions. It is usual to specify a minimum allowable wind speed for the model.

Recommendation 4

When using a Gaussian-plume model the modeller must be able to demonstrate that, for the situation being modelled, the:

a) limitations inherent in the steady-state formulation are not exceeded (the specific factors that should be considered are detailed in Recommendation 3)

b) technical parameterisations in the plume model adequately treat the situation to be modelled.

Figure 2.2 shows the most common and simple Gaussian-plume approach to dispersion modelling. This describes the bell-shaped (Gaussian) distribution of concentrations in the horizontal and vertical directions.

The Gaussian-plume formula provides a better representation of reality if conditions do not change rapidly within the hour being modelled (i.e. conditions are reasonably steady and do not deviate significantly from the average values for the hour being modelled). The Gaussian-plume representation of dispersion described above is simplistic and, as such, should only be applied under certain conditions.

However, it is impossible to prescribe in advance the exact conditions under which a Gaussian-plume model is applicable. The modeller should initially be guided by the recommendations in this Guide and later by experience. A careful examination of model results should be carried out to determine how realistic the output concentrations are at critical times, given the known geography and meteorology. In this sense, the assessment of model results may be more important than the initial choice of model.

Recommendation 5

Gaussian-plume models are generally applicable when:

a) the pollutants are chemically inert, a simple first-order mechanism is appropriate, or the chemistry may be carried out as a post-processing step

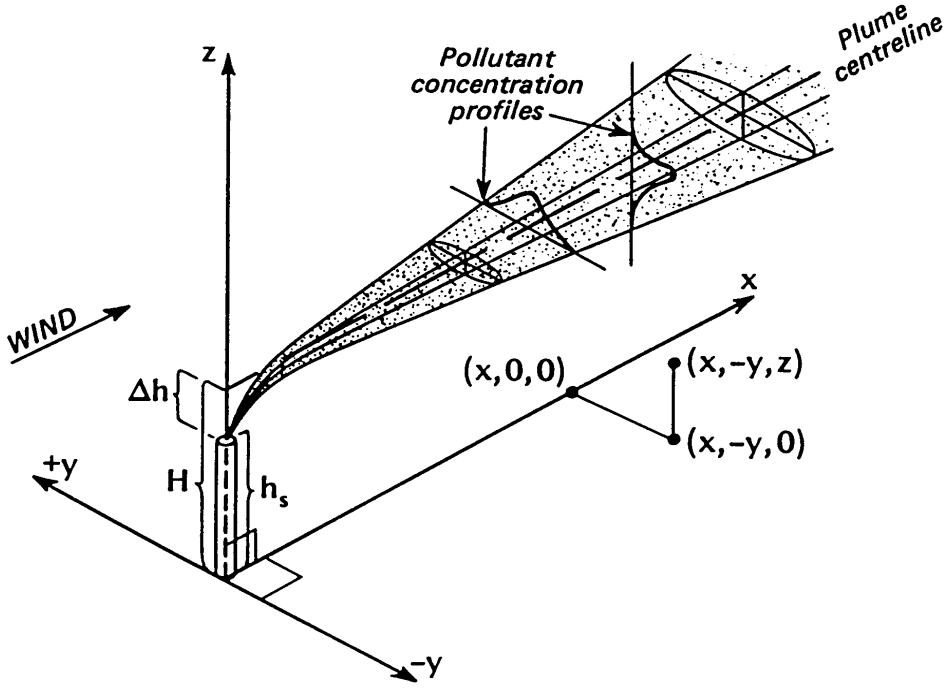
b) the terrain is not steep or complex

c) the meteorology may be considered uniform spatially

d) there are few periods of calm or light winds.

A careful choice of Gaussian-plume model is needed if the effects of deposition, chemistry or fumigation need to be simulated.

Figure 2.2: A typical plume from an elevated point source



Note the plume rise (Δh), and the normal (Gaussian) distribution of pollutant concentrations in the horizontal and vertical (after Oke, 1987).

2.1.1 Common features of Gaussian-plume models

Characteristics of steady-state Gaussian models that make them convenient tools include the fact that they:

- do not require significant computer resources – they can be run on almost any desktop PC and can usually process a complete year of meteorological data in a matter of minutes
- are easy to use – they come with user-friendly graphical user interfaces (GUIs) and a relatively small number of input variables are required
- are widely used – well developed knowledge due to many users and results can easily be compared between different studies
- have simple meteorological data requirements – an input data set can be developed from standard meteorological recordings, and commercially developed data sets are readily available for a number of the metropolitan areas of New Zealand (see Appendix B)
- have conservative results for short (<100 m) or low-level sources – overseas validation shows these models are more likely to over- rather than under-predict ground-level concentrations, which offers some degree of safety in the regulatory environment when assessing discharges from short or low-level sources.

2.1.2 Meteorological data requirements

Although plume models do not have large meteorological data requirements, the meteorology is a crucial component, and good-quality data are needed, ideally from a monitoring site within the area of interest. This is not prohibitively expensive, and is far preferable to using data from a more distant site. This is discussed in detail in section 5.2.

2.1.3 AUSPLUME and ISCST3

Until the last few years, and even currently, AUSPLUME (which was derived from ISCST2) has enjoyed the status of being the de facto standard Gaussian-plume model in New Zealand. ISCST3 is also commonly used in New Zealand, but to a lesser degree than AUSPLUME. Both models are and will remain particularly useful as screening models (which can be used to determine whether more advanced modelling is required or not), and for small, steady-state, near-field applications.

AUSPLUME employs a GUI through which the user may easily edit and execute the model. The model is very easy to use and quick to run, and the output is easily interpreted. The latest version of the AUSPLUME model (version 5.4) has a number of enhancements such as the PRIME building-downwash component.

However, AUSPLUME (and to a lesser degree ISCST3) has been used in some applications without consideration of whether it is the most appropriate model. This is especially true in odour modelling (Godfrey and Scire, 2000) and in other larger-scale, longer-range, complex terrain and non-steady-state-type applications.

AUSPLUME has recently undergone a major re-write. However, despite this upgrading, AUSPLUME (v5) will still be limited in its application because of the fundamental steady-state assumption that it employs.

Despite this widely recognised limitation, AUSPLUME and ISCST3 still enjoy regulatory status in Australia and the United States, respectively.

AUSPLUME and ISCST3 are principally designed for calculating impacts in regions of flat terrain. The more advanced AERMOD and CTDMPLUS are designed for use when complex terrain is an issue. Whether designed for flat or complex terrain, Gaussian-plume models are best used for near-field applications where the steady-state meteorology assumption is most likely to apply.

2.1.4 AERMOD

AERMOD is a 'near-field, steady-state' guideline model. It uses boundary-layer similarity theory to define turbulence and dispersion coefficients as a continuum, rather than as a discrete set of stability classes. Variation of turbulence with height allows a better treatment of dispersion from different release heights. Also, dispersion coefficients for unstable conditions are non-Gaussian, to represent the high concentrations that can be observed close to a stack under convective conditions.

AERMOD was developed in 1995, reviewed in 1998 and formally proposed by the US EPA as a replacement for ISCST3 in 2000. However, this status has not yet been achieved and is likely to take some time.

2.1.5 CTDMPLUS

CTDMPLUS is a US EPA regulatory model developed specifically for tall point-sources in areas of complex terrain. CTDMPLUS is a steady-state plume model containing algorithms that enable a more physically realistic description of vertical dispersion and air-flow around complex terrain features. In the past CTDMPLUS has been successfully used in New Zealand, but it is not frequently used any more due to its highly specialised meteorological data requirements and its applicability only to tall point sources. CTSCREEN (EPA4) is a screening version of CTDMPLUS.

2.1.6 Limitations of Gaussian-plume models

The following limitations of steady-state Gaussian models should be considered and weighed up against the advantages before employing this type of model in any dispersion study.

a Causality effects

Gaussian-plume models assume pollutant material is transported in a straight line instantly (like a beam of light) to receptors that may be several hours or more in transport time away from the source. They make no account for the fact that wind may only be blowing at 1 m/s and will only have travelled 3.6 km in the first hour. This means that plume models cannot account for causality effects. This feature becomes important with receptors at distances more than a couple of kilometres from the source.

b Low wind speeds

Gaussian-plume models 'break down' during low wind speed or calm conditions due to the inverse wind speed dependence of the steady-state plume equation, and this limits their application. Unfortunately, in many circumstances it is these conditions that produce the worst-case dispersion results for many types of sources. These models usually set a minimum wind speed of 0.5 or 1 m/s and sometimes overwrite or ignore input data below this with this lower limit.

c Straight-line trajectories

In moderate terrain areas, these models will typically overestimate terrain impingement effects during stable conditions because they do not account for turning or rising wind caused by the terrain itself. CTDM and SCREEN are designed to address this issue.

d Spatially uniform meteorological conditions

Gaussian steady-state models have to assume that the atmosphere is uniform across the entire modelling domain, and that transport and dispersion conditions exist unchanged long enough for the material to reach the receptor. In the atmosphere, truly uniform conditions rarely occur. Water bodies, hills and other terrain features, differences in land use, surface characteristics, and surface moisture (e.g. irrigated vs unirrigated agricultural fields) all produce inhomogeneities in the structure of the boundary layer which can affect pollutant transport and dispersion.

Convective conditions are one example of a non-uniform meteorological state that Gaussian-plume models cannot emulate. For tall stacks (>100 m) under convective conditions – overseas studies have shown that under prediction can occur in the near field (Hibberd, 2000 and Luhar and Hurley, 2002). The notable exception to this is AERMOD, which has a specially developed, 'add-on' probability density function.

e No memory of previous hour's emissions

In calculating each hour's ground-level concentration the plume model has no memory of the contaminants released during the previous hour(s). This limitation is especially important for the proper simulation of morning inversion break-up, fumigation and diurnal recycling of pollutants over cities.

f A potential quick fix

It is possible to overcome some of the limitations of a plume model without using a complete advanced model run. One potential approach is to use single-surface meteorological data (i.e. AUSPLUME/ISC type files with an advanced model). An example of using CALPUFF meteorological data from a single site ('screening mode') is given in *Analysis of the CALMET/CALPUFF Modelling System in a Screening Mode* (US EPA 1998). Detailed technical advice on how to run CALPUFF using AUSPLUME/ISCST3 type meteorological files is provided in the CALPUFF manual.

However, it should be pointed out that in this screening mode, the benefits of spatially varying meteorology and complex terrain effects are not being taken advantage of. The screening mode is not recommended by the developers of CALPUFF. They suggest that better-quality results can be achieved using CALMET/CALPUFF run with a proper representation of the terrain and three-dimensional meteorological fields.

Recommendation 6

If a Gaussian-plume model is inappropriate for a particular application because of its limitations, and a full puff model meteorological data set is not available, an advanced model with a single-point meteorological data set should be considered.

2.2 Advanced dispersion models

Although Gaussian-plume models are commonly used in New Zealand for regulatory impact assessments, other less restrictive dispersion models are available. These have been in use for scientific research for decades, and are now beginning to enter the regulatory arena. Their use avoids most of the limitations associated with steady-state models. Although their demands on resources (human, computational and data) are far higher than those of Gaussian-plume models, computer power is also increasing rapidly, making this aspect less of an issue. However, the use of advanced models does involve much greater meteorological input data demands.

Advanced dispersion models may be grouped into three categories depending on the way the air pollutants are represented by the model.

Particles

Pollutant releases, especially those from point sources, are often represented by a stream of particles (even if the pollutant is a gas), which are transported by the model winds and diffuse randomly according to the model turbulence. Particle models are computationally expensive, needing at least 10^5 particles to represent a pollutant release, but may be the best type to represent pollutant concentrations close to the source.

Puffs

Pollutant releases can also be represented by a series of puffs of material which are also transported by the model winds. Each puff represents a discrete amount of pollution, whose volume increases due to turbulent mixing. Puff models are far less computationally expensive than particle models, but are not as realistic in their description of the pollutant distribution. However, they are often more than adequate, and are used for regulatory purposes.

Grid points

Pollutant distributions are represented by concentrations on a (regular) three-dimensional grid of points. This is the cheapest formulation computationally, but difficulties arise when the scale of the pollutant release is smaller than the grid point spacing. This method is commonly used for airshed modelling (section 3.1), and the simulation of chemical transformations is most straightforward in a grid model.

Efforts to increase computational efficiency while still retaining a realistic description of pollutant dispersion mean that many models are a combination of the above-mentioned types. For example, the 'PARTPUFF' approach (Hurley, 1994) represents the pollutants as Gaussian puffs in the horizontal and particles in the vertical, particle models usually convert particles to a gridded distribution when the particles have dispersed sufficiently (Lyons et al., 1994), and grid point models often represent sub-grid-scale releases as particles or puffs (Morris et al., 1992).

The fundamental difference between advanced models and Gaussian-plume models is that the advanced models require three-dimensional meteorological fields (see section 4.6) rather than measurements at a single point, and an assumption of spatial uniformity.

There are a number of issues to consider when applying an advanced dispersion model to an air quality assessment. These may deter a potential user, due to the extra investment of effort required, but should lead to more realistic and reliable results. These include:

- a detailed understanding of boundary-layer meteorology, atmospheric turbulence, mesoscale meteorology and (perhaps) atmospheric chemistry and particle dynamics
- a high-specification desktop PC with more memory, disk space and processing time than required for Gaussian-plume models (output files are usually in the order of megabytes and run times can reach hours or days)
- a complex user interface because of more input parameters, which means visualisation of output can also require post-processing software to handle large output files

- an increased risk of model misuse because of the small base of understanding and expertise created by fewer people using advanced models compared to Gaussian-plume models
- a fully three-dimensional, time-dependent meteorological data set is usually required, which needs a good understanding of air pollution meteorology (section 5.3).

However, not all assessments will require a full three-dimensional, spatially varying meteorological data set, and under some circumstances a simple plume model meteorological data set can be used effectively with a puff model run in screening mode. See section 2.1.6(f) for an example of how this may be undertaken.

Recommendation 7

Advanced models should be used when:

a) meteorological conditions vary across the modelling domain and therefore are not compatible with a steady-state model

b) sources or receptors are located in complex terrain, which affects the meteorological as well as the plume-dispersion characteristics

c) pollutants accumulate in calm conditions or are re-circulated as the wind changes direction

d) frequent periods of low wind speed or calms are experienced in the area.

e) chemical transformations between pollutant species are important

f) appropriate meteorological data are available to drive them.

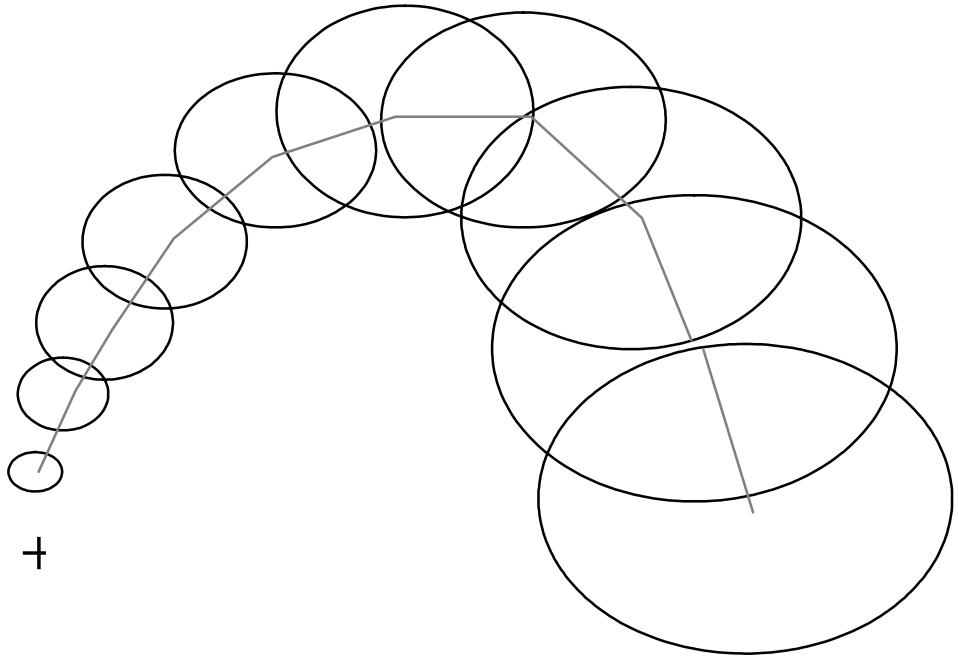
The most commonly used advanced dispersion models in New Zealand are CALPUFF and TAPM.

2.2.1 CALPUFF

CALPUFF (a puff model) has recently been accepted by the US EPA as a guideline model to be used in all regulatory applications involving the long-range (>50km) transport of pollutants. It can also be used on a case-by-case basis in situations involving complex flow and non-steady-state cases from fence-line impacts to 50 km. It is freely available and is the most widely used puff model in New Zealand. For more detailed information and model availability, visit www.src.com/calpuff/calpuff1.htm.

CALPUFF is a multi-layer, multi-species non-steady-state Gaussian puff dispersion model which is able to simulate the effects of time- and space-varying meteorological conditions on pollutant transport (Scire, 2000a). Its puff-based formulation is described in Figure 2.3. This enables the model to account for a variety of effects such as spatial variability of meteorological conditions, causality effects, dry deposition and dispersion over a variety of spatially varying land surfaces, plume fumigation, low wind-speed dispersion, pollutant transformation and wet removal. CALPUFF has various algorithms for parameterising dispersion processes, including the use of turbulence-based dispersion coefficients derived from similarity theory or observations.

Figure 2.3: Graphical representation of the puff modelling approach



\+ Release point

The meteorological data for a full CALPUFF run are provided by CALMET, its meteorological pre-processor. This is described in section 5.3.1. However, it is possible to overcome some of the limitations of the plume model without carrying out a full CALPUFF run, as CALPUFF may also be driven by meteorological data from a single site in the same form as the data for AUSPLUME or ISCST3. This overcomes some of the following limitations of the Gaussian-plume formulation:

- the effects of causality will be simulated (i.e. no spot light effect)
- the previous hour's emissions are included
- calm and low wind speeds will be treated more realistically.

2.2.2 TAPM

The Air Pollution Model (TAPM) was developed by scientists at Australia's Commonwealth Scientific and Industrial Research Organisation (CSIRO) to simulate three-dimensional meteorology and pollution dispersion in areas where meteorological data are sparse, or non-existent (Hurley, 2002). The formulation of TAPM enables it to run quickly, therefore long-term simulations can be carried out on a PC – similar meteorological models generally need fast workstations. The modelling system contains a number of dispersion modules. These include a particle/puff dispersion model for dispersion from point, line, area and volume sources, and a three-dimensional grid-point model for urban air pollution studies. The dispersion models allow for plume rise and building wake effects, and wet and dry deposition, and there is a chemistry module for urban airshed applications. One feature of TAPM is that the meteorological file for the modelling run is created automatically using meteorological information and terrain data supplied for the model. For more detailed information and model availability, visit www.dar.csiro.au/tapm. TAPM's performance has been verified for several regions in Australia, and the model system is being used at several institutions in New Zealand.

The applications that TAPM and CALPUFF are designed for are very similar, as both are intended for regulatory impact assessments (among other things). They are a significant advance on the steady-state Gaussian-plume formulation. Their main difference is in the calculation of the meteorological fields used by the dispersion model. This is discussed further in section 5.3.

2.3 The relative cost of advanced dispersion modelling compared to Gaussian-plume modelling

There is anecdotal evidence to suggest reluctance among practitioners to use advanced dispersion models because of potential additional costs. Cost is an issue that needs to be considered when contemplating which approach to adopt for an assessment. However, it is difficult to compare the different approaches quantitatively because of the number of issues that influence the overall cost of the modelling exercise, which are outlined below.

- **Staff upskilling** – the time and cost involved in this will be more because of the complexity of advanced modelling.
- **The detail of source and site data** – this is similar to other modelling methods.
- **Meteorological and terrain data** – producing a full meteorological data set and terrain file requires more input data and takes more time than for a plume model. There are several options for minimising the cost of this. If the terrain is not complex then it may be possible to produce good results using a plume model meteorological data set. If a full meteorological data set is required, it may be more efficient to purchase a ready-made data set if available. Several organisations are currently developing these data sets. An alternative is to seek independent expertise to produce the required data.
- **Configuring model and processing time** – initially, configuring an advanced dispersion model is likely to take more time because of the large number of variables associated with this type of model. As a modeller becomes familiar with the more complex modelling system, the difference in effort required by the two systems is not likely to be significant. Running an advanced model will take more computer time, but because the models can be run on desktop PCs there is little or no cost difference between running a puff and a plume model.
- **Interpreting and reporting the model output** – all modelling approaches require similar levels of time and cost to interpret and report the model output, and so there is no significant cost difference here.
- **Credibility of results** – this is likely to be regarded more highly, and the cost of processing an industrial assessment of environmental effects (AEE) minimised, if the model is not operating outside the limitations for which it was designed. In circumstances where the use of an advanced dispersion model can produce more credible results, there is likely to be a cost benefit in using that type of model.

Recommendation 8

The potential benefits of producing more credible results should be weighed against the disadvantages (including cost) of using an advanced dispersion model before deciding which approach to take in a particular dispersion study.

2.4 Limitations of advanced dispersion models

Advanced dispersion models are more sophisticated than Gaussian-plume models, and aim to produce more realistic results. Even so, results from advanced models should *not* be automatically assumed to be better than those gained from Gaussian-plume models. One situation where this situation may arise is when a feature that has been added to a plume model (e.g. a building downwash algorithm) is not included in advanced models.

Some other examples where advanced models may do no better than Gaussian-plume models include:

- grid-point models close to a localised source
- near-field receptors under non-convective conditions
- near-field receptors for wind speeds over 1 m/s.

Depending on the situation being modelled, the choice between representating the pollutant release as a plume (i.e. Gaussian-plume models) or a collection of puffs or particles (i.e. advanced models) may be less important than incorporating atmospheric chemistry or deposition or dense gas effects, which a particle model may not include.

The issues that will determine whether or not advanced models will provide more realistic results will vary from case to case. As a starting point, a comparison of the manuals and validation studies of both (or all) the models being considered should provide the modeller with some guidance on whether or not better results could potentially be obtained by using an advanced model.

In summary it is important to:

- remember that results from advanced models should *not* be automatically assumed to be better than Gaussian-plume models
- clearly justify the choice of model being used.

3 Specialised Applications of Dispersion Modelling

The dispersion models discussed so far are principally concerned with assessing the effects of specific sources on specific locations. Their key features are:

- the sources are well identified (although there may be quite a lot of them)
- they can be point, line or area sources
- the impact locations are specified
- they are usually focused on worst-case circumstances (or at least identifiable cases leading to some specific undesirable effect).

This section provides an introduction to a number of specialised dispersion models which to date have not been frequently used for regulatory purposes. However, with the ongoing development in the number and type of effects that are required for an assessment of environmental effects (AEE), these models are likely to be used more often in the future.

3.1 Airshed modelling

In many circumstances, particularly in urban areas, we want to know about the effects of all the sources of emissions on a whole area. Standard dispersion models (whether Gaussian-plume or puff) cannot do this very well, so a different class of model is applied – the airshed model. In theory, provided all the sources can be identified, a standard dispersion model could perform the task, but in most cases the number of sources is too large for the model to handle and the computing resources required would exceed the capacity of most desk-top computers.

3.1.1 What is airshed modelling?

Rather than tracking the plumes of contaminants from point (or line, or area) sources, an airshed model divides the whole region of interest into a series of cells, and models what happens as contaminants are moved by the wind from one cell to the next. Airshed models also include formulations of the chemistry of the atmosphere, so they can account for chemical transformations that occur in the atmosphere.

The models have variable grid sizes and time steps, depending on the requirement. These can range from very large-scale models, with grid cells of hundreds of kilometres examining air quality parameters over entire continents for many years, to micro-scale models, with grid cells of a few tens of metres and time steps of a few minutes.

Airshed models also need to take account of what is happening in the vertical structure of the atmosphere and thus have a number of layers in the grid boxes, often with variable depth. These range from a few metres deep (particularly in the lower layers close to the ground) to hundreds of metres deep. The depth almost always includes the boundary layer (up to a few km), but in some larger-scale models needs to cover the entire troposphere (up to 30 km).

As for dispersion models, airshed models require two key types of input information: emissions and meteorology.

a Emissions

The emissions of all contaminants of interest, including anything they might react with, needs to be known for each grid cell and time step. This is no simple task, even for small, uncomplicated areas. Therefore a reasonable emissions inventory is required, identifying all sources from point, area and line emissions including domestic, mobile and natural (particularly vegetation) sources. In-depth information about how to calculate and compile the emissions from a particular airshed is provided in the *Good Practice Guide for Preparing Emission Inventories* (Environet, 2001).

Before compiling the required emissions data, the following choices need to be made. Some of these can require considerable resources to quantify.

- **Spatial resolution** – 1 to 3 km is typical. Higher resolution is desirable, but the number of grid cells, effort required to identify emissions, and computer time needed to run any model increases dramatically.
- **Time resolution** – the ideal is hourly. However, it is often impractical to explicitly determine many emissions on an hourly time frame. In these cases sub-models can be used. For instance, mobile emissions can be estimated using a traffic model, or vegetation emissions from a broad understanding of the daily and seasonal cycle of plant growth.
- **Contaminants** – these depend on the application, but most models would require CO, SO_2, NO_x and particulates, plus a good description of volatile hydrocarbons. Most models include NO_x and ozone, and these are intimately involved in most chemical reactions of contaminants. These reactions are strongly influenced by volatile (or reactive) hydrocarbons. Some models require these to be known to great accuracy, with each compound specified, and over 100 can be involved. Other models can perform adequately by using a single estimate of reactive hydrocarbon emissions. Commonly used photochemical transformation mechanisms include:
  - SAPRC 99 (http://pah.cert.ucr.edu/~carter/SAPRC99.htm)
  - Carbon Bond IV (i.e. http://airsite.unc.edu/soft/cb4/cb4main.html
  - RACM (http://pah.cert.ucr.edu/~carter/epacham/stockwel.pdf)
  - Generic Reaction Set (http://www.dar.csiro.au/pollution/IER_Calc/IERdescription.htm#Azzi_1992).
- **Period to model** – this depends on the application and computer power, with two periods being typical. The first is examining a case study over one to three days, with the objective of understanding the response of the airshed to a particular event (e.g. a high ozone day). The other is over periods of a year or longer, examining trends and scenarios.

b Meteorology

In addition to the emissions, meteorology is also a strong determinant of air quality, so a good description of the meteorology is vital because the effects are cumulative. Unfortunately, however, meteorology is often the most uncertain input into airshed modelling assessment.

Consider two grid cells in close proximity, both with high emission rates. If wind speed and/or direction are not known accurately, then the emissions from one grid cell can either add to or miss the other completely. This can result in errors of up to ±100% in the total concentration of emissions. If this situation is extended to a number of grid cells, or to a complex meteorological case with re-circulation, the errors can become enormous.

A similar situation arises if we do not know enough about the vertical structure of the atmosphere. Consider two extreme cases: firstly, a light-wind day with a very stable atmosphere, and perhaps an inversion at 100 m; and secondly, a light-wind day with a good mixed layer 1000 m deep. The model will mix contaminants through this layer, and the concentration difference in these cases – which are entirely realistic – is a factor of 10.

Meteorological fields for use in airshed models are usually derived from a specialised mesoscale meteorological model, which can be part of the airshed modelling system or a completely separate component.

3.1.2 Where is airshed modelling used?

Airshed models are used to examine the air quality characteristics of entire regions, incorporating all the relevant features of the region. The region, or airshed, is defined by the application.

For some purposes the airshed might be quite small, as when looking at a single contaminant in a valley, without major chemical reactions such as carbon monoxide or particles from wood burners. In this case the sources might be well known, the chemical reactions negligible, and the meteorological cases of interest straightforward. In the extreme, this case could lead to the application of a highly simplified form of airshed modelling, the 'box' model, which has just a single grid cell into which all contaminant emissions are mixed.

A more common application of airshed models is for an urban airshed, which is from a few kilometres to tens of kilometres. In this case, it is desirable to know all the emissions from a city, where they are going, and what affect they have on the air quality of the city and surrounds.

Larger-scale applications such as modelling the airshed of entire states or countries are not used in New Zealand. These are often used for photochemical pollution studies, or to assess acid rain, where transport of hundreds of kilometres is relevant. Such models are used extensively in Europe, Asia and the US. The most extreme airshed is the whole hemisphere.

3.1.3 What information do airshed models provide?

Model outputs contain a huge amount of information. Imagine a typical, realistic, upper-end domain of a 100 km x 100 km grid with 1 km spatial resolution, ten vertical layers, run for a year with one-hour time resolution, specifying eight typical contaminants. This is 7 gigabytes of data, and if printed out would be a stack of pages slightly higher than Auckland's Sky Tower.

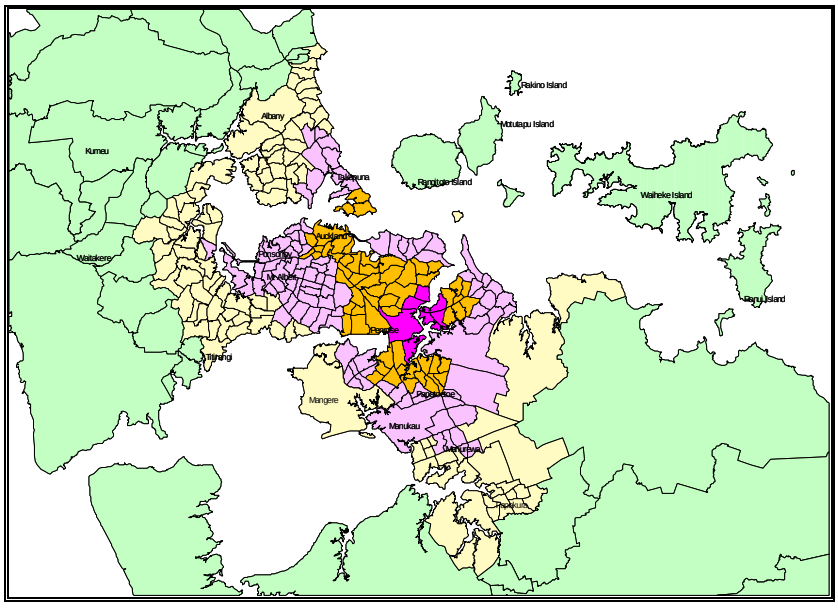
Key statistics, multi-dimensional charts, time series at selected points and short-term case study periods are all necessary to display and assimilate airshed model outputs. The choice depends very much on the application. Some example applications are provided in Table 3.1.

Table 3.1: Some example applications for airshed modelling

Frequently asked questions	Method
"What's the peak value occurring, and where and when?"	A global search on the output files will determine this easily.
"Where should we locate our monitors to make sure we get a representative picture of air quality in the area?"	A visual examination of a selected series of maps of ground level concentrations will provide a good indication.
"What will happen if we allow vehicle emissions to double?"	Select either areas, or times, with peaks, and re-run the model with the extra emissions.
"What effect will an unusually warm summer have on our air quality?"	Alter the meteorological file appropriately and re-run.
"We can't monitor the air quality at all of our schools, but can we get an idea of what sort of air quality they experience through a typical year?"	For each of the school locations, print out a time series of the contaminant of interest.
"We need to know people's exposure as part of a health study – can we get a map of average and peak concentrations?"	For a suitable-length model run, produce GIS maps of the relevant statistic.
"I've got an idea about what causes poor visibility on some days, but do we have any information on chemicals in the air above the ground?"	Produce maps or time series of the contaminant in the relevant layer.
"What is the effect on urban air quality of new industrial sources?"	Run the airshed model with and without the new emissions.

An example model output for epidemiological exposure research in Auckland is shown in Figure 3.1. This shows the relative exposure to NO_2 in July 1999 by analysing airshed model output and counting the number of occurrences of NO_2 above a pre-specified level. This information can help to determine how many people are affected by different levels of pollutants and hence what the likely health effects are.

Figure 3.1: Map of Auckland showing the relative public exposure to NO_2 in July 1999 by census area unit



Although running an urban airshed model is a fairly specialised task, the final example in Table 3.1 is an important one in the context of the effects of new point sources. The effects of new NO_x emissions cannot be considered in isolation from those already present, because the production of NO_2 from NO is limited by the amount of ozone present, which must be 'shared' between all sources. Consequently, the NO_2 produced by the new source – if considered to be geographically isolated – will be overestimated compared to the extra NO_2 produced by that source in the presence of other emitters. If the new source is close to a complex system of air pollution emitters (e.g. a traffic network), then it is more realistic to apply an airshed model to the whole system as part of the resource consenting process for the new industrial source. The need for an assessment of the 'regional' effects of new industry has already arisen in New Zealand.

3.1.4 What models are available for airshed use?

A large number of airshed models are continually being developed. Some examples are mentioned here.

UAM-V (Urban Airshed Model – variable grid) is one of the most common airshed models and was developed by Systems Applications International (SAI). It is available free from SAI or through the EPA website (www.epa.gov/scram001) and can be downloaded in executable form with all supporting guidance documentation (http://www.uamv.com/). It performs reasonably well, but is not particularly user-friendly and requires a great deal of effort to run. UAM has undergone continual development over the last decade and in many ways is now a more advanced model than other more recent models. It has numerous modules and a complex structure.

CALGRID is an increasingly popular model, developed by EarthTech Inc. It is freely available from either EarthTech or the California Air Resources Board website (http://www.arb.ca.gov/eos/soft.html#calgrid), and is more user-friendly. It links to its companion model, CALMET, which produces a realistic meteorological file (the dispersion model CALPUFF is also part of the series). CALGRID is easier to install and run, but still needs a focused effort to obtain the appropriate emissions inventory files and links to a good meteorological file. CALGRID is used in New Zealand, and has been applied to Auckland successfully.

The US EPA has recently released the Models-III photochemical-aerosol modelling system (http://www.epa.gov/asmdnerl/models3/cmaq.html). This is a complex, multi-scale modelling system which comprises an emissions inventory, prognostic meteorological modelling and chemical transport-transformation modelling sub-systems. The CMAQ (Community Multi-scale Air Quality) is the main component of the system, modelling the processes of pollutant transport, chemical transformation and wet and dry deposition for a variety of primary and secondary gaseous and aerosol species.

TAPM (http://www.dar.csiro.au/tapm/index.html) has recently been coupled with the CSIRO chemical transport model that includes a highly condensed chemical transformation mechanism. This enables more complex chemical transformation mechanisms to be considered and allows TAPM to be usefully applied to modelling inter-seasonal and inter-annual variations in photochemical smog concentration. TAPM has been applied in Auckland, Christchurch, Timaru and Nelson.

A number of companies offer 'commercial' airshed models or, more commonly, complete packages which provide a specific deliverable. These are usually achieved by the use of an in-house model specifically developed by the company.

There are also a large number of 'research' grade models. These are not discussed here, because many are highly specific to the issue being studied, or are too complex for third-party users.

Recommendation 9

Airshed (rather than point-source) models should be used when assessing the air quality characteristics of entire regions, incorporating all the relevant features of that region.

Airshed models should be used to:

a) design and assess management programmes
b) examine long-term air quality trends
c) provide air quality information where there is no monitoring data
d) provide data for use in exposure assessments
e) assess the effects of new sources in urban areas, when their emitted pollutants interact chemically with those from sources already present.

Identify and include all emissions from point, domestic and area, mobile and natural sources (particularly vegetation), into the airshed model.

Calculate and compile the emissions using methods consistent with the guidance provided in *The Good Practice Guide for Preparing Emission Inventories* (Environet, 2001).

The New Zealand Traffic Emissions Rates Model (Ministry of Transport, 2000) should be used to provide data for vehicle emissions.

Airshed models require three-dimensional, time-dependent meteorological fields, which may be obtained from a specialised mesoscale meteorological model or extrapolated from local monitoring site data (see section 5.3 on meteorological inputs for advanced models).

3.2 Roadway emissions modelling

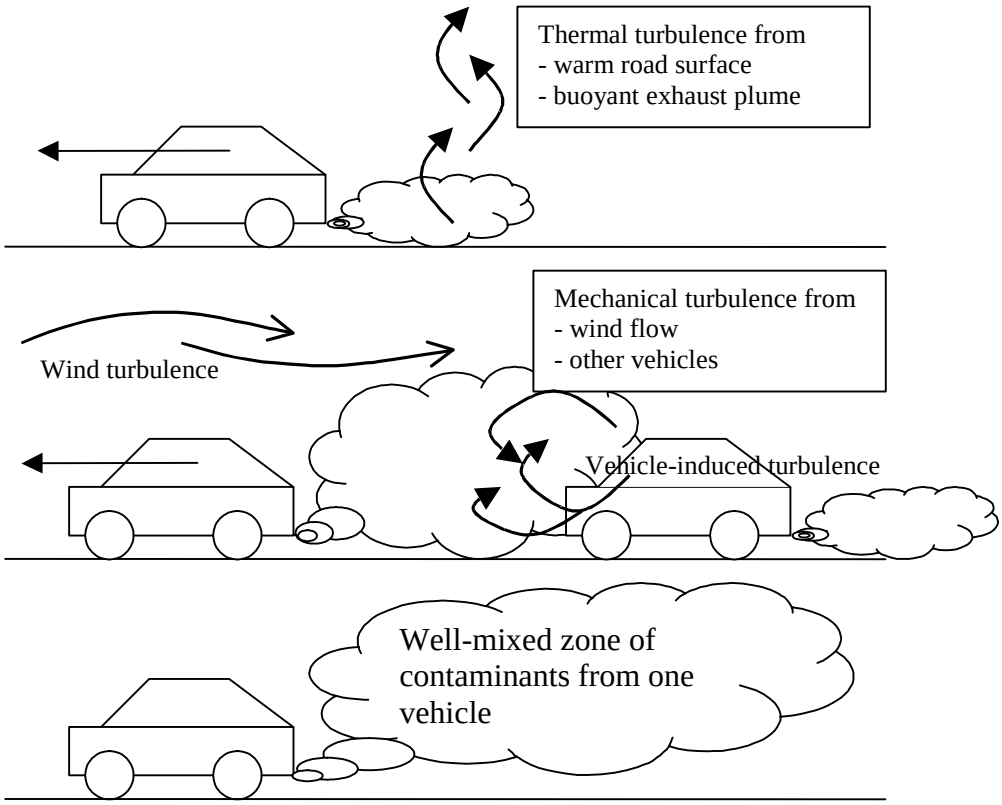
Until recently the adverse effects of proposed roadways on air quality have not been considered in New Zealand. The Ministry of Transport and Ministry for the Environment commissioned a study to identify the key factors affecting roadside pollution concentrations and to predict pollutant concentrations near roadways in New Zealand in 1997. The report, *Transport Emissions Study – Modelling and Monitoring* (Ministry for the Environment, 1997), provides a good introduction to the effects of roadway emissions in New Zealand. This report can be downloaded from http://www.mfe.govt.nz/publications/air/transport-emissions-study-sep97.html.

Assessing the effects of emissions from vehicles and their transport and transformation at the urban scale is complex. Atmospheric dispersion modelling is one tool used internationally to assess the impact of proposed roadway developments.

3.2.1 What is roadway modelling?

Figure 3.2 is a schematic representation of the emission and mixing processes associated with vehicle emissions. Thermal and mechanical turbulence occurring behind a vehicle contributes to mixing the emissions, so that the air behind a vehicle is relatively well-mixed. If the situation described in Figure 3.2 is expanded to show a flow of vehicles travelling both ways along a road, a 'line source' of contaminants is developed. In many situations the modelling of roadway emissions is carried out using a Gaussian-plume model configured to emulate the dispersion of contaminants from this type of line source.

Figure 3.2: The effect of thermal and mechanical turbulence combining to produce a well-mixed zone of contaminants



Obtaining an accurate emission rate is critical to the success of any modelling project. Estimating the type and quantity of contaminants emitted from roadways is inherently complex because emissions vary according to:

- the driving cycle (e.g. accelerating, steady speed, decelerating, idling)
- roadway conditions (e.g. free flow or congested)
- vehicle fleet composition
- traffic volume.

Because of these complexities, roadway modelling often requires an emissions model to meet the input data requirements of the model. In New Zealand the Ministry of Transport has funded the development of a vehicle emissions database, New Zealand-Traffic Emission Rates (NZ-TER). Details and the availability of NZ-TER are described at: http://www.mot.govt.nz/publications/14_26doc.shtml.

Users of NZ-TER have raised a number of issues to be aware of when using the model, including:

- emission factors being based on a small number of tailpipe tests
- emission factors only including tailpipe emission – no fugitive or non-tailpipe emissions are accounted for
- NZ-TER includes a number of undocumented assumptions (e.g. future vehicle fleet compositions and the rate of adoption of emission control technology)
- the unquantified but most likely significant effect of badly maintained or otherwise high-pollutant-emitting vehicles – although these vehicles comprise the minority of the fleet they may account for the majority of traffic-related emissions.

To date NZ-TER has not been peer reviewed or validated against real world monitoring data. The Ministry of Transport is currently working towards having NZ-TER peer reviewed. In addition to this, NIWA plans to use data collected on the tailpipe emissions from 40,000 vehicles in Auckland to validate the emission rates calculated by NZ-TER.

The Ministry of Transport has also produced a New Zealand Rail Emissions Inventory, which is available upon request.

3.2.2 What roadway models are available?

Dispersion modelling is widely used for assessing the effects of roadway emissions in Europe, England and the United States. Information about the commonly used roadway models can be found at the following internet sites:

- US EPA – http://www.epa.gov/scram001/index.htm (choose dispersion models)
- UK Department of Environment, Food, and Rural Affairs – http://www.defra.gov.uk/environment/airquality/laqm/guidance/pdf/laqm-tg03.pdf
- European Environmental Agency – http://155.207.20.121/mds/bin/allmodels.

EPA Victoria (Australia) has recently released the dispersion model AusRoads, a simple line-source Gaussian-plume dispersion model for predicting the near-road impact of vehicle emissions. The methodology is based on the US CALINE4 model. Although the functionality of the original CALINE4 near-road model has been retained, AusRoads has been written so that data entry is easier and a number of artificial limitations have been removed. For example:

- AusRoads has increased the number of links and receptor locations that can be modelled
- a full year of local meteorological information can be read into the program from an external file
- road geometry, traffic density and emission factors and receptor location information can now be entered either directly from the graphical user interface or read from external files.
- AusRoads is available from EPA Victoria (www.epa.vic.gov.au).

3.2.3 An example of a roadway model: CALINE4

This section illustrates some of the important generic issues associated with roadway modelling using the California Line Source Model (CALINE4) as an example. This model is commonly used in New Zealand, the USA and England, is quite user-friendly and is freely available. CALINE4 is only one of many roadway models available. Other well-used models include CAR-FMI (Karppinen et al., 2000) and AEOLIUS (UKMO, 1995).

CALINE4 was developed by the California Department of Transportation and the US Federal Highways Agency for assessing roadway traffic emissions. It is based on the Gaussian diffusion equation and employs a mixing zone concept to characterise dispersion over the roadway. CALINE4 is a Gaussian-plume model and as such is subject to the same limitations of other steady-state Gaussian-plume models (see section 2.1.6).

CALINE4 can model roadways, intersections, street canyons, parking areas, bridges and underpasses. Each CALINE run allows the prediction of up to eight one-hour mean concentrations. Therefore it is useful for investigating one-hour concentrations of NO_2 and CO and eight-hour concentrations of CO.

The US EPA lists CALINE4 as the preferred/recommended roadway model (US EPA, 1999). The UK Department of the Environment, Transport and the Regions lists CALINE4 as an advanced model (UK DETR, 2000) but does not indicate any form of approval or endorsement.

a Where can I get CALINE4?

The source code, GUI and manual are available free at:
http://www.dot.ca.gov/hq/env/air/calinesw.htm

b What input data does the model need?

CALINE4 requires the user to define:

- hourly meteorological conditions
- line-source emission rates
- number of vehicles
- roadway configuration
- receptor locations.

c What care needs to be taken when using this model?

CALINE4 requires meteorological data of a similar type and format to other Gaussian-plume models such as ISCST3 or AUSPLUME. However, unlike other dispersion models, the CALINE4 GUI will only allow eight hours of meteorological data to be processed during each run. The modeller must therefore choose a ‘worst case’ set of meteorological conditions. Identifying this will take some experimenting with the meteorological input data. In addition to this, the maximum ground-level concentration for each receptor is likely to occur under different meteorological conditions. Run times longer than eight hours can be achieved if the model is run in batch mode via the DOS prompt.

The estimation of roadway emission data is a very important but complex task. The New Zealand-Traffic Emission Rates (NZ-TER) database is considered more likely to estimate emissions accurately from the New Zealand vehicle fleet than using overseas emission factors, because the New Zealand vehicle fleet contains a unique mix of vehicles, emission control standards and fuel-type uses.

The Gaussian formulation used in CALINE4 is based on two somewhat restrictive assumptions:

1) horizontally homogeneous wind flow, and
2) steady-state meteorological conditions.

Complex topography can bring the validity of each of these assumptions into question. For these reasons, use of CALINE4 in complex terrain should be approached with care.

CALINE4 is a steady-state model and is not designed to emulate the changing rate of emissions from decelerating, idling and accelerating vehicles (i.e. the emission rate for each roadway element in the model is an hourly average). To accurately assess the effects of vehicles passing through an intersection, careful consideration of fluctuating emission rates associated with decelerating, idling and accelerating becomes important. While CALINE4 contains an intersection module it may be more appropriate to use an intersection-specific model such as CAL3QHC (CALINE3 with queuing and hot spot calculations). The source code, GUI and manual are available free of charge, and can be found under Screening Tools at http://www.epa.gov/scram001/index.htm.

Unlike many other dispersion models CALINE4 does not allow gridded receptors to be used. The user can define a maximum of 20 receptors. The location of these should be set to assess exposure at the most sensitive sites and in the approximate locations where maximum impacts are likely to occur (e.g. at the down-wind end of long straights).

3.2.4 Future developments in roadway modelling

Modelling roadway emissions is developing in parallel with other fields of atmospheric dispersion modelling. The trend is towards non-steady-state models that will more accurately emulate dispersion in complex situations such as within complex terrain or street canyons. Three examples of advanced roadway models are:

- Operational Street Pollution Model OSPM (Fu et al., 2000)
- SPRAY (Nanni et al., 1996)
- HYROAD (Ireson and Carr, 2000)
- Lagrangian wall model (LWM) (M. Cope, CSIRO Atmospheric Research, Australia).

The Lagrangian wall model (LWM) solves a similar set of chemistry equations to those in a complex chemical transport model (CTM). The two-dimensional wall is moved at the speed of the vertically averaged wind, allowing considerable speed-up of the solution of the model equations. This allows the model to be operated at very high resolution (10 m), making it suitable for modelling near-road air quality impacts. Initial concentrations in the ‘wall’ (upwind of the road or sources of interest), and boundary conditions at the edges of the wall, are obtained from the CTM or a model such as TAPM, albeit at a larger scale. Alternatively, the boundary conditions can be merely specified as a typical background concentration.

At the time of publication the Ministry is considering the development of further detailed national guidance on assessing discharges to air from transport. Such guidance would be prepared in conjunction with the Ministry of Transport and the Auckland Regional Council. In the meantime, the following recommendations are offered as guidance.

Recommendation 10

Specialised roadway models should be used when assessing the effects of contaminants discharged from transport corridors.

The currently available roadway models should only be used in non-complex terrain.

When calculating an emission rate of a contaminant from a particular roadway consider the following factors:

a) traffic volume

b) vehicle speed

c) vehicle fleet composition

d) roadway conditions (e.g. free flow or congested).

Use the vehicle emissions database, New Zealand-Traffic Emission Rates (NZ-TER). If an alternative is employed, specifically justify this.

Take care to identify the worst-case meteorological conditions that will generate the maximum ground-level concentration for each receptor.

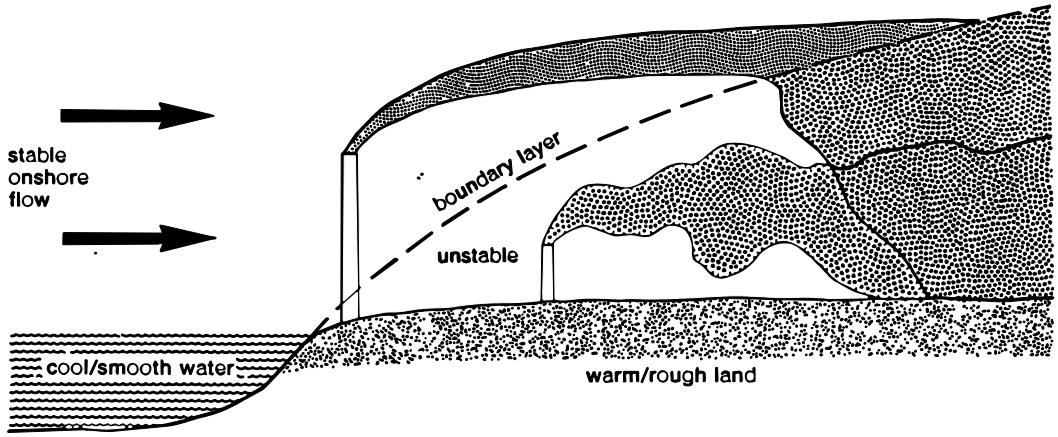
If assessing the effects of discharges from vehicles passing through an intersection, consider using a model that accounts for the variation of emissions with driving cycle (e.g. accelerating, steady speed, decelerating, and idle).

The meteorological and emission input data for roadway models require a different approach to that used more commonly in point-source modelling.

3.3 Modelling coastal fumigation

Consider a tall stack, located on a shoreline, which emits a narrow plume towards land (Figure 3.3). The plume is embedded in the stable boundary layer and is intercepted by a growing thermal internal boundary layer (TIBL) over land. The height of the TIBL increases with solar heating of the land surface. Convective mixing over land can rapidly bring the elevated pollutants to the ground, causing local high ground-level concentrations. Unlike the fumigation events associated with the erosion of nocturnal ground-based inversions (see section 4.5.7c), coastal fumigation may persist for several hours, and in the same location.

Figure 3.3: Coastal fumigation



Coastal fumigation is an important issue in Western Australia, for example. The effects have not been observed to the same degree in New Zealand because the substantial flat land mass and relatively deep, cool water needed to generate this effect are not as common here as in continental land masses. However, the potential effect of coastal fumigation should be considered carefully if you are dealing with a large source located on a coastline. DISPMOD, a steady-state Gaussian-plume model developed by the Western Australia Department of Environmental Protection, and the US EPA model OCD (Offshore and Coastal Dispersion), contain algorithms to model TIBL effects and may be appropriate tools if coastal fumigation is identified as a significant issue at a particular site.

Other steady-state models cannot simulate the high ground-level concentrations in the TIBL. However, advanced models, such as CALPUFF and TAPM, which give more realistic representations of the meteorology in the coastal area, are arguably the most suitable for simulating the fumigation process.

Recommendation 11

When modelling the dispersion of pollutants from a source located near the coast, the effects of coastal fumigation may be simulated in either:

a) a Gaussian-plume model, which has the ability to handle this specific effect (e.g. DISPMOD, OCD, ADMS3 or US EPA's SCREEN 3); or

b) an advanced model, which gives a realistic representation of the meteorology in the coastal area.

3.4 Visibility modelling

Visibility is a good measure of how humans perceive the atmosphere. It is measured by how far people can see and what colour the sky is, and is therefore an amenity value rather than a health hazard. Predicting how visibility will be degraded is complex because it involves estimating not only the dispersion of contaminants but also the way they are transformed by reactions in the atmosphere and how people perceive visibility. For more information on managing and monitoring visibility in New Zealand, refer to the *Good Practice Guide for Monitoring and Management of Visibility in New Zealand* (Ministry for the Environment, 2001c).

Atmospheric physicists and chemists have developed and produced a number of tools that enable modellers to study visibility degradation at several spatial scales. CALPUFF is the US EPA regulatory model for regional visibility modelling. PLUVIEW is the US EPA regulatory model for calculating the visual impact of a single plume. The FOG model for calculating the visual impact of a single plume is built into the CALPUFF model.

In New Zealand, there is no specific visibility monitoring programme and no attempt to quantify any future risks using modelling. It is, however, recognised that visibility is an environmental issue in this county (Ministry for the Environment, 1999). The sources of visibility degradation are many and complex, ranging from wind-blown sea spray to dust, fine particles, gases, haze, rain, fog and clouds. Visibility modelling in New Zealand is still in its infancy and is only performed for research.

Recommendation 12

To model the effect of emissions on visibility:

a) use the approach and models recommended by the US EPA as a starting point
b) consider the influence of site-specific (i.e. New Zealand) conditions.

3.5 Dispersion modelling on larger scales

Atmospheric processes and air pollution dispersion phenomena are commonly classified with regard to their spatial scale. The most common use of dispersion models in New Zealand is to predict near-field effects that occur within 10 km of the source. The effects of urban-scale air pollution can often be observed at greater distances; for instance, the Auckland urban plume reaching the Coromandel Peninsula, or the Christchurch urban plume reaching the southern Canterbury and Otago regions. In such complex cases, advanced models must be used – the straight-line steady-state Gaussian-plume model in a uniform wind field is simply too unrealistic. The same types of models are used for all scales from urban upwards; it is largely only the processes – meteorological and pollution dispersion – that may differ.

3.5.1 The regional scale

The regional scale may be defined as having characteristic distances of between 10 and 1000 kilometres. At this scale, airflow is influenced by thermal and dynamic effects such as flow channelling and the variation of the region's energy balance with land use, vegetation type and water bodies. This scale is commonly referred as the 'mesoscale' when discussing meteorological features, and their importance for pollution dispersion must be considered when choosing a model for regulatory impact assessments.

Usually, the simulation of mesoscale, or regional pollutant, dispersion must be carried out by advanced meteorological and dispersion models. Only at the small-scale end of the range might a Gaussian-plume model be appropriate.

All prognostic meteorological models – referred to simply as 'mesoscale models' – and their associated dispersion models are applicable for regional-scale simulations (e.g. for cases in which dispersion over the whole of New Zealand is important). CALMET (Scire et al., 2000b) and CALPUFF are also suited to this application if there is good meteorological data coverage over the domain of interest. CALMET can also be driven by meteorological output from mesoscale models if data are sparse. On a regional scale the production of secondary pollutants (e.g. ozone and fine particles) becomes more important, and so atmospheric chemistry cannot be ignored.

Recommendation 13

To model the dispersion of pollutants on a regional scale:

a) use prognostic meteorological models and their associated dispersion models
b) consider the transformation of pollutants due to atmospheric chemistry.

3.5.2 Long-range transport

At much larger scales, with distances of, say, more than 1000 km, meteorology is governed by large-scale pressure-gradient forces and the rotation of the earth. This scale includes weather systems such as anticyclones, depressions and fronts, although the effects of these feed into the mesoscale and smaller scales. Long-range transport may be thought of as dispersion on these 'continental' scales, as controlled by weather systems. It is important when considering, for example, trans-boundary transport across mainland Europe, the transport of pollutants from the USA across the Atlantic Ocean to Europe and, occasionally, the transport of air pollution from Australia across the Tasman Sea to New Zealand (e.g. smoke from fires around Sydney).

All regional modelling systems can be used for long-range transport, provided they can account for the Earth's curvature in their co-ordinate systems, and the chemical transformations that occur on the associated (extended) timescales.

Long-range transport models are used to provide information on the transport and fate of emissions from locations such as the UK to Europe or from state to state in the USA. The chemistry in these models is very important, as pollutants are both removed and chemically converted with distance from the source. Some examples of long-range transport models are STEM (Carmichael et al., 1991), ATMOS (Arndt and Carmichael, 1995), CRIEPI (Ichikawa and Fujita, 1995) and NAME (Ryall and Maryon, 1998). Another well-known model in Europe is RAINS (Regional Air Pollution Information and Simulation), which was developed as a tool for the integrated assessment of alternative strategies to reduce acid deposition in Europe and Asia (Alcama et al., 1990). This model describes the pathways of emissions of SO_2, NO_3, HNO_3 and NH_4, and explores their impact on acidification and eutrophication. The use of long-range transport models has not been explored in New Zealand.

3.6 Accidental releases

Accidental releases can result in very high ground-level concentrations of pollutants, albeit for a short time period. A number of accidental releases are of particular concern. A catastrophic rupture of a pipeline or tank, or a spill from a tank, can produce a release that lasts from a few seconds to a few minutes. This results in a burst of material or a puff-type release. Gases or liquids may leak from around seals, pipe joints and valves, or from cracks or holes in vessels. This type of release may start slowly and increase in size. High-pressure releases of both gases and liquids from pressure relief valves or pressure seal ruptures could occur, and may be accompanied by flashing of the fluid to a vapour-liquid mixture. If a release lasts from 10–30 minutes, it could be described as a small continuous release.

Modelling accidental releases may be required for a variety of reasons.

For long-term industrial site planning – modelling could be used to see the effects of different accidental release scenarios, and thereby help to determine the terrain, meteorology and surrounding residential areas most favourable for the prevention of significant harm to the residents.

To identify the types of accidental releases that could result in significant downwind adverse effects – this would enable prevention planning through the design of mitigation equipment and emergency planning through evacuation strategies. This type of modelling is also used as a consequence tool for risk assessment.

These models are also used by emergency response services if an accidental release does actually occur. The model outputs are used to identify potentially affected people and estimate requirements for evacuation.

Modelling accidental releases requires both a source emission model (because of the nature of accidental releases, you can not measure them), as well as a transport and dispersion model. It is important to know whether the discharge involves gases that are heavier than air (known as dense gases). Many accidental releases do involve dense gases that cannot be modelled by the commonly used plume or puff models. Dense gases require specialised treatment from dense gas models such as DEGADIS+ (US EPA, 1998c), SLAB (Ermak, 1990) or AUSTOX (Ross 1994; Ross and Koutsenko, 1993).

ALOHA (Areal Locations of Hazardous Atmospheres) is one of the most commonly used accidental release models and is used worldwide for response, planning, training and academic purposes. ALOHA uses information provided by its operator and physical property data from its extensive chemical library to predict how a hazardous gas cloud might disperse in the atmosphere after an accidental chemical release. ALOHA can predict rates of chemical release from broken gas pipes, leaking tanks and evaporating puddles, and can model the dispersion of both neutrally buoyant and heavier-than-air gases. ALOHA is intended for use during hazardous chemical emergencies and was designed to be easy to use so that inexperienced responders can use it during high-pressure situations. Further detail on ALOHA can be found on the US EPA's CAMEO (Computer Aided Management of Emergency Operations) website (http://www.epa.gov/ceppo/cameo/techdes.htm).

Recommendation 14

When there is an instantaneous release or a burst of buoyant material, a puff model like CALPUFF (version 6) can be used.

When modelling accidental releases, choose a tool that is capable of handling the specialist requirements associated with this task.

When planning emergency response procedures, extra care must be taken to accurately calculate the emission and dispersion of these contaminants because of the potentially high (perhaps even lethal) impact of accidental releases.

When modelling an actual accidental release a fast response emergency response will obviously be required. In this instance, an approximate but conservative estimate of the area potentially affected by the release is appropriate.

Readers can refer to Schnelle and Dey (1999) for more information on modelling accidental releases.

3.7 Salt and steam effects: cooling towers

Steam effects are visible steam plumes from cooling towers, such as those found at power stations and petroleum product refineries. The central North Island of New Zealand is a large geothermal area where geothermal power stations are often located next to major roadways. Fogging from plumes released by geothermal cooling towers frequently occurs (Godfrey and Fisher, 1994), and modelling is often used to determine if the plume could cause visibility problems for motorists or aircraft.

Salt effects may be caused if a steam plume contains salts (from the use of salt water in the cooling tower). They can be detrimental (in the long term) to vegetation and can also enhance the corrosion of building materials.

When modelling for the visual extent of a plume, the model calculates the plume path, length and radius under a particular set of emission and environmental conditions and includes assessment of parameters such as liquid water content and the plume/environment temperature difference. An example of a visual plume calculation model is ATCOOL, a standard fogging model developed by Dr Steven Hanna of the US EPA. ATCOOL is used to calculate the variation of cooling-tower plume parameters with height and distance downwind. Plume-length calculations from ATCOOL have been well validated by observations at many locations.

Spray-water drift deposition assessment can be carried out using the SACTI model, developed by the Argonne National Laboratory for the Electric Power Research Institute (EPRI) in California, USA. SACTI contains a number of models, which include drift deposition, visibility and shadowing. Which is to say, SACTI is not just a drift deposition model. This model is capable of calculating the amount of water deposition that can occur from droplets of spray out of cooling towers. This requires an assumption of a drift rate (a rate that water is emitted) and a typical droplet size distribution. The model has strict input data requirements for accurate humidity and vertical profile information because model results are extremely sensitive to humidity. If there are contaminants in the water droplets, such as salt, deposition rates for those contaminants can also be calculated by assuming a concentration of the contaminant in the droplets.

FOG was a stand-alone model but its algorithms have now been incorporated into the CALPUFF model. CALPUFF is designed to simulate the transport and diffusion of water vapour emissions from multiple point sources and is set to become the default US EPA model. See http://www.epa.gov/scram001/ for more details.

Recommendation 15

To model salt and steam effects:

a) use the approach and models recommended by the US EPA as a starting point.

b) consider the influence of site-specific (i.e. New Zealand) conditions.

4 Getting Started

4.1 Where does it come from?

Models attempt to simulate a real situation using mathematics. The types of physical situations that result in the release of pollutants to the atmosphere are classified as types of 'sources', with user-specified characteristics. This section details the criteria used by the models to describe the characteristics of the sources being modelled.

4.1.1 Physical characteristics

There are four main types of sources used in dispersion modelling (Figure 4.1):

- **point source –** discharges from a small opening such as a stack or vent
- **area source –** a source with a large surface area, such as a landfill surface, contaminated site, a pile of solid material, or a liquid surface (pond, tank, lagoon)
- **line source** – a long, narrow source such as a roadway, conveyor belt, or roofline vent along a long, narrow building (usually a line source must be redefined as a chain of volume sources for modelling)
- **volume source** – bulky, diffuse source such as emissions from within a building.

Some models (e.g. TAPM) allow various types of gridded emission sources to represent complex emission inventories, and can include emissions from many different anthropogenic and biogenic/natural sources.

The ISCST3 model also includes a special algorithm for modelling concentration and deposition impacts of particle emissions from open pit sources, such as surface coal mines or rock quarries.

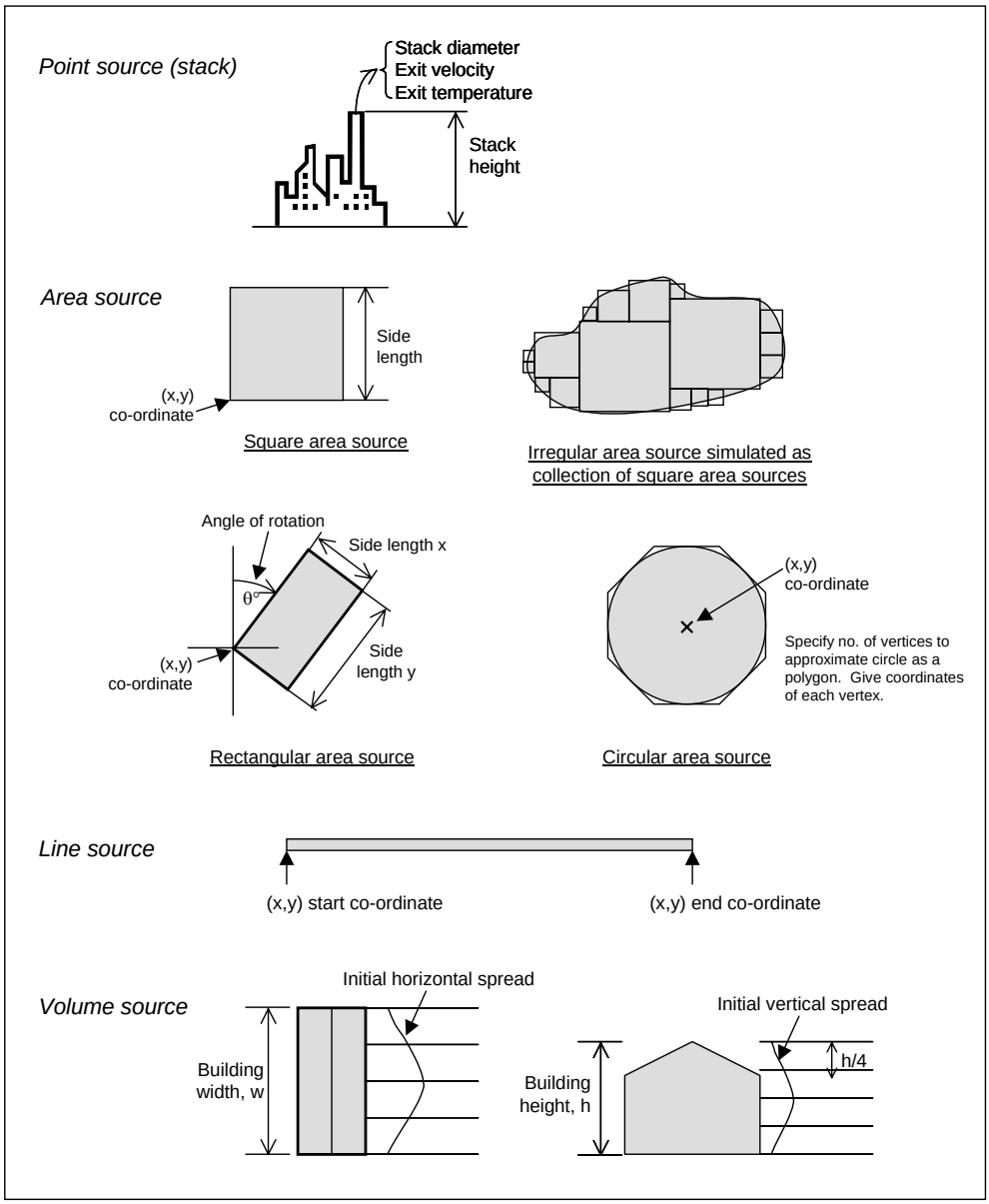
a Point sources

Point sources require the specification of emission temperature and exit velocity in addition to emission rates. The importance of exit velocity is discussed in section 4.1.4. AUSPLUME requires temperature data in degrees Celsius, and ISCST3, CALPUFF, AERMOD and TAPM require temperature data in Kelvins.

If you want the emission temperature to be the same as the ambient temperature in the meteorological data file, as when your stack is discharging building ventilation air at the same temperature as the atmosphere, then in ISCST3 set the emission temperature to 0 K, as this defaults the model to use the ambient temperature. In AUSPLUME, if the emission temperature is below the ambient temperature, the model will round the emission temperature up to the ambient temperature. So if you want the emission to discharge at ambient temperature, set the emission temperature to be lower than the lowest ambient temperature in the meteorological file. However, this will cause an error if the ambient temperature is lower than 0°C as the model cannot handle an emission temperature lower than 0°C.

Special care must be taken when modelling sources that are not point sources. Figure 4.1 illustrates a number of different source types. The model will specify the source as a release of plumes or puffs, which have Gaussian concentration distributions. The model will automatically assign 'effective' locations of the initials plumes/puffs and their horizontal and vertical spreads – these are not necessarily the actual location or size of the physical source (but are, of course, closely related). This means that, in general, modelled concentrations close to the source are not realistic, as the true source is represented as a series of Gaussian-shaped plumes or puffs. To circumvent this, and obtain realistic near-source concentrations, the physical source should be divided into smaller elements. For instance, a roadway is divided into segments, each represented by a point source in the Gaussian-plume model CALINE-4 and similar models.

Figure 4.1: Types of sources used by dispersion models



b Area sources

Some models assume that individual area sources have square dimensions. In practice, sources are usually irregular in shape. You can approximate these irregular shapes by using an appropriate selection of a number of square area sources. However, AUSPLUME 5, ISCST3 and CALPUFF also allow area sources to be rectangular, circular or polygons with irregular angles. The rectangular area sources can be rotated to any angle rather than oriented parallel to a north-south grid.

For square area sources, the models handle area sources as a line source that rotates to maintain its crosswind orientation. In this sense, the area source more closely resembles a circular source than a square. The initial vertical dispersion is calculated as if it were a distance L metres upwind (where L is the area source side length) in order to simulate the diffusion that occurs as the pollutant moves across the source. Receptors should not be located closer to an area source than the area source's width (VicEPA, 2000). Estimating concentrations close to the source may require several smaller sources to be used to represent the actual source.

The models use a numerical integration approach for modelling impacts from non-square area sources. While this option is slower, it allows more exact estimates to be made close to the source (VicEPA, 2000).

CALPUFF allows for thermally buoyant area sources. This may be significant if the area source is much hotter than the ambient temperature, such as a tank containing hot trade wastes from an industrial process or a surface fire. Although AUSPLUME and ISCST3 do not calculate thermal buoyancy effects from area sources, it is possible to estimate the effective release height using standard buoyancy flux equations. The model may then be run with the source at the effective height and at actual height to give an envelope of concentrations. (Note this treatment is only applicable for small area sources. Large, hot area sources such as open burning, detonation of explosives and/or bushfires should be addressed using source-specific models. For more information, refer to the US EPA SCRAM website www.epa.gov/scram001/). In most cases however, the area source will be at a temperature close to ambient, and thermal buoyancy effects will be negligible.

Terrain effects and building downwash effects are *not* computed for area sources in either AUSPLUME, ISCST3, CALPUFF or TAPM.

c Line sources

Line sources are not modelled by AUSPLUME and ISCST3, and must instead be treated as volume sources (see section 4.2.1d). In AERMOD, line sources are represented as a string of volume sources or elongated area sources. In CALINE-4, line sources are divided into strings of point sources. Buoyant line sources are modelled by CALPUFF and TAPM.

d Volume sources

The size of volume sources is specified using initial horizontal and vertical spreads. These depend on the type of volume source and what the source is representing (such as a ridge-line vent), and can be obtained from tables in the user's guide or online help system for each model.

A common application of a volume source is to model the fugitive emissions escaping from a building. Here, the initial vertical and horizontal plume spreads may be taken as a quarter of the building height and width respectively (VicEPA, 2000). This assumes that the bulk of the material (about 86%) is captured in the building wake. To be conservative, the building width should be taken as the minimum of the building dimensions. In this example, the model creates a virtual source so the emissions are released at half building height.

To model a line source, a row (or arc) of volume sources must be arranged along the centreline of the real line source with separations less than about one-quarter of the distance to the nearest receptor. Results will then be insensitive to the value chosen for the horizontal spread of the volume sources, although a recommended distance is half of the separation between volume sources. The vertical spread should be set as one-quarter of the line source's height. Since line sources adjacent to a building are affected by the building wake, the volume sources should be located along the building centreline with initial vertical spreads equal to one-quarter of the building height.

Building downwash effects are not computed for volume sources in either AUSPLUME, ISCST3, CALPUFF or TAPM. Terrain effects are computed for volume sources.

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.

Recommendation 16

Select the most appropriate source type offered by the model. Justify the source type selection if it is not obvious.

Use measured (or planned) dimensions and characteristics to describe the source.

If the dimensions and characteristics of the source are not accurately known or have not been calculated, run both a worst-case scenario (i.e. the configuration of source that results in highest ground-level concentration) and the most likely realistic dimensions. Present and compare the results of both scenarios.

Consider using an alternative model, or even a different form of assessment, if a particular source does not fall easily into one of the source types that a particular model is designed to handle.

4.1.2 Emission rates: the number one critical parameter

Emission rates can be a major source of error and inconsistency in any modelling analysis. For inert pollutants, the modelled concentration is directly proportional to the emission rate, so any errors in the emission rate data translate directly into errors in the model results. It is therefore important to use emission rates that are as accurate as possible.

Sources of emission data include:

- measurements from a particular (or similar) source
- manufacturer's specifications or process information
- published data (e.g. US EPA's AP-42 database)
- regulatory authority files and data
- calculated emissions from emission models (e.g. NZ-TER).

Emission rate data should ideally be sourced from measurements undertaken at either the site in question (for an existing site) or a similar site (if available). A significant number of emission tests have been undertaken at different sites in New Zealand and so there is a substantial amount of local emission data available. Regional councils are probably the best source of this data.

Alternatively emission rates may be calculated from manufacturer's specifications or directly using industrial process knowledge.

When no appropriate measured emission rates are available, published emission factors can be useful. Published emission factors give the mass of pollutants discharged per mass of fuel consumed, or product processed, and are useful as a first estimate of emission rates for pollutants where collection of actual emission rate measurements is impractical or impossible. Examples of these include the US EPA's AP-42 Emission Factors (www.epa.gov/ttn/chief/) or the UK Emission Factors Database (www.naei.org.uk/emissions/). Australia employed a set of 82 calculation handbooks for the National Pollutant Inventory, largely based upon US EPA emission factors. These handbooks are available at www.npi.gov.au.

New Zealand has its own database for calculating transport emissions. This is the NZ-Traffic Emission Rates (NZ-TER), and is available at http://www.mot.govt.nz/publications/14_26doc.shtml. This is discussed further in section 3.2.1

Emission factors are typically assigned a rating to reflect their accuracy. The accuracy rating and the applicability of any emission factor to New Zealand conditions must be considered and should be discussed when used in any study.

Consider using a different form of assessment if the emission rate from a particular source cannot be confidently measured or accurately calculated.

For simple dispersion model scenarios with only one or two sources, the maximum measured emission rate from the source(s), or the calculated emission rate corresponding to maximum production or fuel burning rate, is typically used for dispersion calculations.

Special care is required where there are several sources of a pollutant on one industrial site. In most cases all discharges are unlikely to emit their highest emission rates simultaneously, resulting in high ground-level concentrations. In such cases, it is more realistic to model all the sources together using some kind of average or variable emission rate for each source (section 4.1.3). Each source should also be modelled individually using its worst-case maximum emission rate to determine its maximum potential effect. If a few sources are likely to discharge worst-case emissions at the same time, such as in the case of a treatment system upset at a sewage plant or a cyclone failure at a processing plant, then all of those sources should be modelled together at their maximum emission rates. If this is the case, be realistic about the number of failures that are actually likely to coincide and provide an approximation of how frequent the failure events are likely to be.

Recommendation 17

When dealing with measured emission rates from a source **with multiple measurements** over a period of time (e.g. a vent monitored on a number of occasions):

a) use the maximum measurement if only a few data points are available (e.g. fewer than 4–5)

b) if a number of data points are available (e.g. greater than 5–10), then draw a curve and use a certain percentile (such as 50th or 70th percentile) emission rate (the percentile should be selected on a case-by-case basis after examination of data). Vic EPA (1985) provides guidance on what percentile values may be useful.

When dealing with measured emission rates from **a large area source**, measurements should be taken at a number of locations over the surface in a short space of time, and a mean calculated which represents the average emission over the surface at that point in time.

When dealing with an **area source that contains separate zones of different emission rates,** each zone should be measured as a separate source and then modelled as such.

4.1.3 Variable emission rates

If your sources exhibit variable emission rates, either over short- or longer-term periods, it may be important to consider programming the model to simulate the variation in the emissions. This would reduce the possibility of the model over-predicting long-term (longer than one-hour) averages, which could occur if the maximum emission rate was assumed to apply for 24 hours per day, 365 days per year.

There are a number of ways in which emission rates may vary. Some of the processes that can drive the need to use variable emission rates are when:

- a process does not operate 24 hours per day
- the rate of process (e.g. rate of combustion or production) varies throughout the day
- when the emission rate (e.g. odour or dust) varies with temperature or season
- the emission is from a large area source where the emission rate varies over the surface
- the emission is from a large liquid area source such as an oxidation pond, where the emission varies with wind speed over the surface.

AUSPLUME, ISCST3 CALPUFF and TAPM allow you to vary the emission rates by:

- hour of day
- hour and season
- month
- wind speed and stability category
- ambient temperature
- hour by hour variation read from an external file.

If you are modelling the discharge from a combustion source such as a coal boiler, where the combustion rate varies throughout the day, remember that emission rates may not decline in proportion with a decline in combustion rate as the combustion efficiency changes, and at lower

combustion rates the efflux velocity and temperature will also change. These factors all have an effect on the rate of dispersion from the stack and should be accounted for (see section 4.1.4).

For some processes, emission rates may vary substantially in a random fashion. An example would be a waste combustion process in which emission spikes of sulphur dioxide or hydrogen chloride will occur unpredictably because of the variable sulphur and chlorine content of the waste fuel. In such situations, using maximum emission rates to estimate maximum short-term concentrations (e.g. hourly averages) is likely to result in gross over-estimation, because there is only a small chance of maximum emissions coinciding with worst-case meteorology. However, it is possible to use probabilistic methods that take into account the frequency distributions of predicted concentrations and emission rates (measured or estimated) to assess the likelihood of maximum emission rates coinciding with unfavourable meteorological conditions.

Detailed descriptions of the application of probabilistic methods to account for the effect of varying emissions rates can be found in Amr Abdel-Aziz and Frey (2003a, 2003b).

Recommendation 18

Use variable emission rate data when:

a) there is evidence that shows how much and how often the emission rate will vary from the maximum potential emission rate as operational conditions change

b) assessing average ground-level concentrations for periods longer than the time that maximum emissions actually occur for

c) assessing the actual rather than the potential frequency of pollution events.

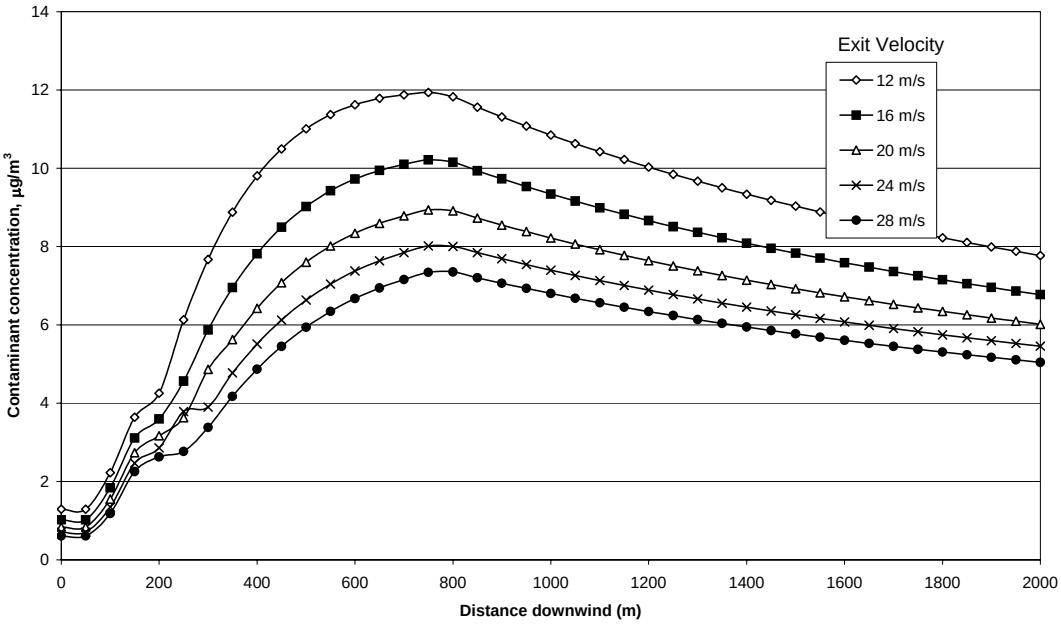
When using variable emission rates, account for other factors that also vary with operational conditions, such as lowered efflux velocities and temperatures.

4.1.4 Exhaust flow – influence of stack hoods

Stacks are modelled as point sources. Parameters that control plume rise, such as the initial vertical momentum and thermal buoyancy of the plume (section 4.3.2), are calculated from the characteristics of the stack emissions, in particular the temperature and exit velocity. If the exit of the stack is not pointed in a vertical direction, and unimpeded by any obstruction, the exit velocity used by the model will be different to the gas velocity within the stack itself. The exit velocity used by a model in this case is the vertical component of the exhaust flow (see Figure 4.3).

An example of the effects of stack exit velocity on dispersion is shown in Figure 4.2. The improvement in dispersion diminishes with increasing exit velocity, and the amount of improvement will vary depending on the stack height. When designing a stack, it is necessary to optimise both the stack height and the exit velocity.

Figure 4.2: Example of the effect of exit velocity on dispersion (stack height = 30m)



If you have a stack which discharges vertically into the air with no impediment to the vertical movement of the exhaust gases, then the exit velocity for the model is simply the volumetric flow of gas (at discharge temperature) divided by the stack-tip diameter. Diameter-reducing cones fitted to the stack tip can be used to increase the exit velocity, although in practice this may not achieve the proportional increase in velocity that you expect. This is because of the increased flow resistance and pressure drop generated by the smaller exit diameter. If the process generating the discharge has fans upstream, the change in pressure drop may change the performance and flow rate of these fans, and bigger fans may be needed. If the process does not have any fans, the change in pressure drop will decrease the flow rate out through the stack, and fans may need to be installed.

It is important when modelling discharges from a stack being fitted with a diameter-reducing cone to account for the increase in resistance and pressure drop (resulting in decreased flow). For example, it would be incorrect to assume that the flows shown in the first two stacks in Figure 4.3 are equal (unless fans were introduced to the second stack). It requires the expertise of process or ventilation engineers to accurately calculate the effect of the introduction of a diameter-reducing cone on exit velocities.

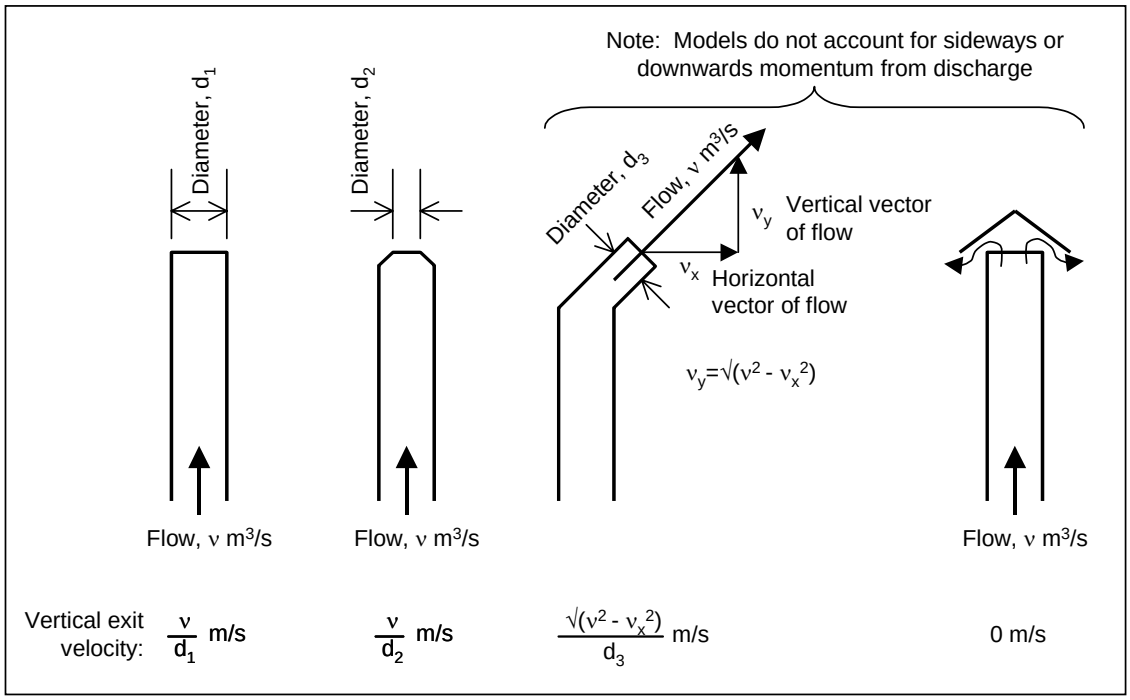
The relationship between fan selection, flow rate and pressure drop is not simple. If you are faced with this situation it will be helpful to seek advice from someone with qualifications and experience in this area.

If you have a stack that discharges exhaust gases at an angle to the vertical, you must calculate the vertical component of the flow vector and use that component as the exit velocity in the model (Figure 4.3).

If the stack has a fitting such as a ‘chinese hat’ to prevent rain ingress, or discharges horizontally or at an angle to the ground, the effective vertical exit velocity is zero. This can have a large effect by reducing the rate of dilution and dispersion. For this reason many regional councils require that this type of rain hat be removed from stacks.

It should be noted that the models do not account for significant sideways or downward momentum from the stack, such as could occur if the discharge is sideways or deflected down by the stack geometry. This will influence ground-level concentrations, particularly for receptors close to the source. This additional uncertainty in the model results should be acknowledged if the results are to be presented in a report. Because of the relatively large uncertainties associated with modelling the dispersion of contaminants from this type of source, it is not advisable to rely on the accuracy of the results. More realistic results may be obtained if the modelling is undertaken using a volume source.

Figure 4.3: Calculation of exit velocity for various stack-tip designs



Recommendation 19

The vertical efflux velocity of a gas stream leaving a stack must be adjusted to account for the influence of any object that may increase resistance to, or change the direction, of the flow.

4.1.5 Multiple sources

Most dispersion models allow you to enter a large number of sources at a time and model the ground-level concentration from each source, either together, separately or in subgroups (called 'source groups'). The models assume that if source A causes a concentration XA at a particular receptor, and source B causes a concentration XB at the same receptor, then the combined ground-level concentration at that receptor is XA + XB. This assumption is valid for pollutants where mass is conserved, such as particles or hydrogen sulphide, but is not valid for odours. More discussion on the applicability of this assumption for odours can be found in the Ministry for the Environment's *Odour Management Guide* (Ministry for the Environment, 2002b).

To improve the quality of modelling results, multiple sources can be used to break up large area sources into smaller sources, such as for the purpose of defining parts of the area source with different emission rates, or for modelling a long chicken shed with a roof vent along its length as a chain of volume sources.

The time required by a computer to carry out the dispersion calculations increases in proportion to the number of sources. In some cases, if you wish to reduce the calculation time, small multiple sources can be grouped and modelled as one larger source. This can be particularly useful if you are modelling a large number of sources and the ones you wish to group together do not dominate the major individual sources (e.g. multiple clarifiers at a sewage plant). In doing so, you must check that your receptors of interest are far enough away from the source so that the model results are not affected by the grouping.

Recommendation 20

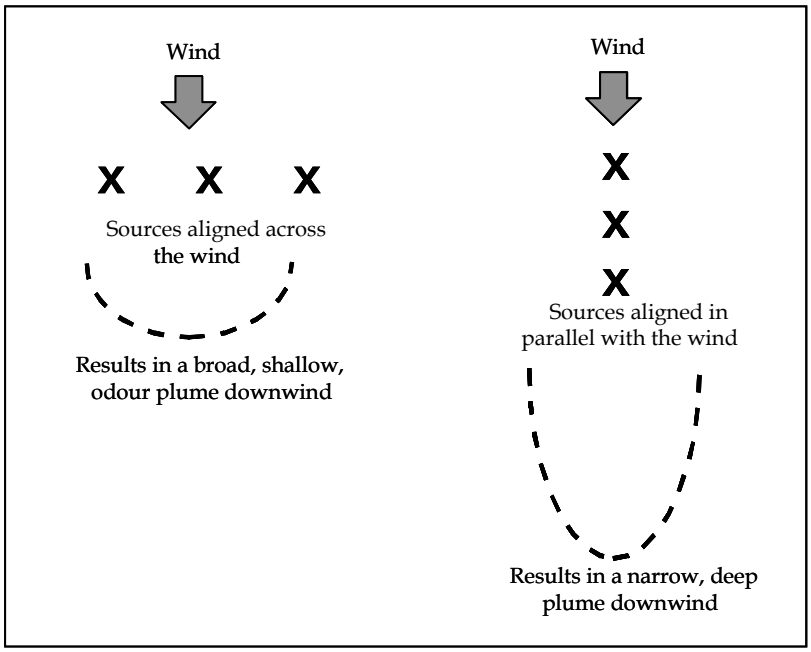
If running a screening model with multiple sources, you must:

a) use a number of screening meteorological data input files that contain different wind directions to determine which will generate the highest concentrations

b) ensure you account for the potential effect of building downwash.

A example of the effect that different source and wind alignments can have on ground-level concentrations is shown in Figure 4.4.

Figure 4.4: Effect of source alignment in dispersion modelling



A stack containing multiple flues, or multiple stacks close together, will have enhanced buoyancy and a higher plume rise, and will therefore generate lower ground-level concentrations than would be the case if the flues or stacks were modelled as separate sources. The effect of enhanced plume rise due to multiple stacks was described and then modelled by Briggs (1975) using algorithms. Manins et al. (1992) demonstrated that plume rise could be enhanced by 10 to 45% by the presence of multiple stacks. Therefore, when modelling a source with a number of stacks in close proximity, unless the effects of enhanced buoyancy are accounted for the ground-level concentrations may be over-predicted. The effect of enhanced plume rise appears to be greatest with large sources such as power plant cooling towers and fossil-fuelled electricity plants. The effect may not be so significant with small or medium-sized sources. Approaches to account for enhanced plume rise have been described by Bornoff et al. (2001), Kong et al. (2002) and Overcamp and Ku (1988).

Recommendation 21

When modelling multiple flues, or multiple stacks that are close together, take account of the effect of enhanced plume buoyancy.

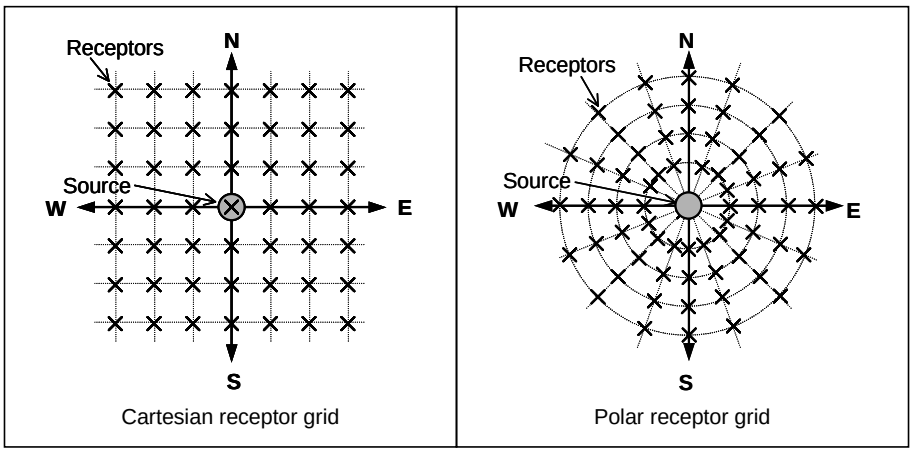
In some cases, the flues may have similar diameters and flow rates. In this case, if the flues are adjacent to one another (within three diameters), enter a stack having the same effective cross-sectional area as the sum of the individual flue cross-sectional areas. Calculate an effective exit velocity though the single flue that gives the equivalent volumetric flow rate to the combined flues.

4.2 Where does it go to?

All dispersion models require the specification of the co-ordinates downwind from a source where the ground-level concentrations are to be recorded. The grid of receptors can be an evenly or unevenly spaced Cartesian or polar grid (Figure 4.5).

Guidelines for defining the extent, spacing, and elevation of a grid are covered in sections 4.2.1 to 4.2.3. Dealing with complex terrain and surface roughness is discussed in section 4.2.4.

Figure 4.5: Cartesian and polar grids

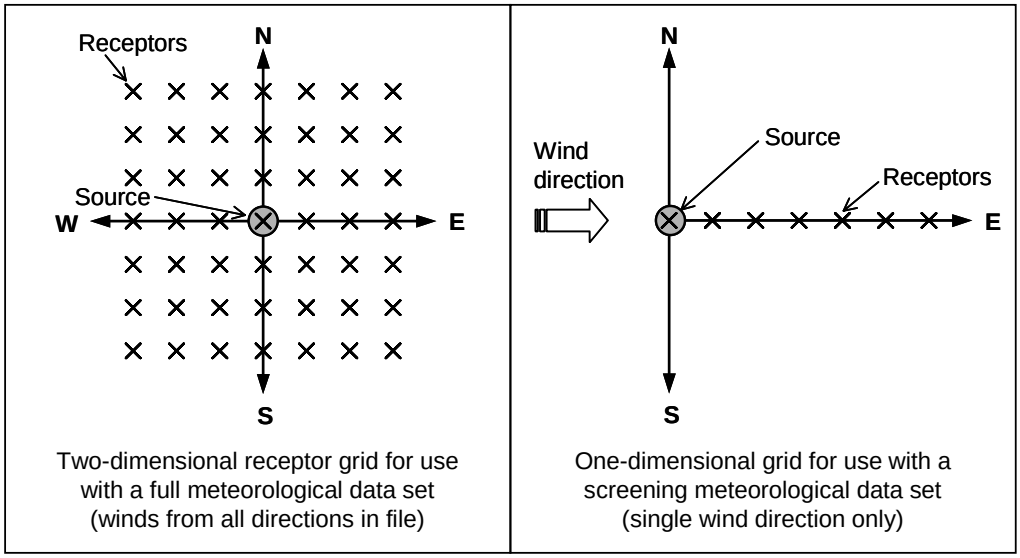


4.2.1 Grid extent

The extent of the grid should be chosen to include any regions of sensitive or important receptors such as residential areas, and should also be sufficiently large to capture peak downwind pollutant predictions. For sources emitting pollutants close to ground level, the maximum ground-level concentration will be close to the source. However, for stack sources the maximum ground-level concentration can be some distance away, and the model may have to be run more than once with increasing grid ranges to make sure the peak is captured.

If the model is being run in screening mode with a single wind direction, the grid extent can be reduced by removing any receptors upwind of the source(s). In addition, if the sources are in line with the wind direction blowing either north-south or east-west, the grid extent can be further simplified by removing all receptors in the cross-wind direction except the one directly downwind of the plume centreline (Figure 4.6). Graphical results plotted from a simplified grid such as this will have a two-dimensional format.

Figure 4.6: One- and two-dimensional grids



If you are using a Gaussian-plume model, you should note the guidelines for range applicability of Gaussian-plume models (section 4.3.1) when defining your grid extent.

Recommendation 22

The extent of the grid must be chosen to include any regions of sensitive or important receptors (e.g. residential areas, schools and hospitals). The spacing and extent should also be configured to capture peak downwind ground-level concentrations.

4.2.2 Grid spacing

Selecting the spacing between individual receptor points is a compromise between processing time and the required results resolution. If you double the number of receptors in your grid, the processing time will also double. However, if the spacing is too large, the peak ground-level concentration may fall between two receptor points and not be captured in the results file.

Recommendation 23

Check that the grid spacing is small enough by running the model with increasingly smaller grid spacings near the location of the peak ground-level concentration, until halving the grid spacing effects a change in peak ground-level concentration of less than 10%.

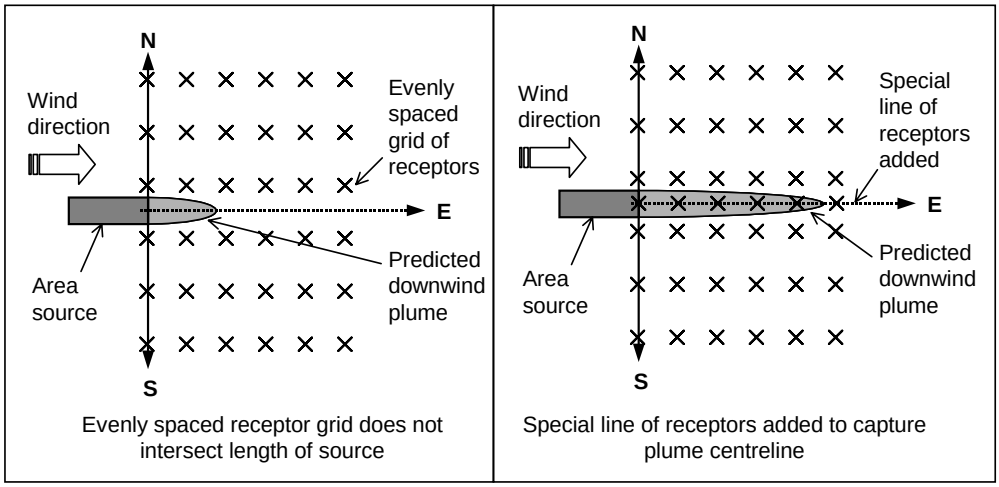
Irregularly spaced grids can be used to concentrate the number of receptors close to the location of the peak ground-level concentration. If the run-time or memory requirements become too great when a grid is subdivided, one solution is to reduce the domain to one or more smaller areas over several runs of the model, then merge the results later. Alternatively, run the model on a coarse grid first, then again on a fine grid with a smaller extent but centred on the area of maximum ground-level concentrations.

If you are using a polar grid, to ensure capture of peak ground-level concentrations round off all wind directions in the meteorological data so that they align with the rays of the polar receptor grid. This only works if all the sources are located at or near the origin of the grid so that the plume's centreline always travels directly over a ray of receptors (or almost so). This adjustment procedure will only provide reasonable ground-level concentration predictions if the emission source is not embedded in elevated terrain, and only if one-hour averages are being compared against guideline limits. In other instances, adjusting the orientation of the wind direction to coincide with polar receptor grid will over-estimate the frequency at which the peak concentration will occur in any one location. In these (more complex) situations a better approach would be to increase the number of rays in the receptor grid rather than adjust the meteorological data file.

If you are planning to use SURFER to plot the results of your model (section 6.1.3), set the number of grid points in the 'Grid Data' option within SURFER to the same as your number of receptors. This will ensure that SURFER graphs the modelled results exactly at each receptor, rather than interpolating different numbers if the concentration is changing rapidly at this location.

Take special care when positioning receptors if you have small or elongated area or line sources. A line of receptors may need to be specially placed parallel to and running through the longest dimension of the source, so that the plume centreline from this source is actually picked up by the model (Figure 4.7).

Figure 4.7: Effect of grid spacing on small or elongated sources



4.2.3 Elevated (flagpole) receptors

Unless otherwise specified by the user, models produce concentrations at ground level. It is standard practice that assessments of pollutant concentrations are conducted at ground level. Some modellers use concentrations that occur at the (approximate) height of a person (e.g. 1.8 m). In reality there is unlikely to be a significant gradient between the concentrations occurring at 1.8 m and at ground level. For the sake of consistency it is recommended that unless specific circumstances require otherwise, assessments are conducted at ground level.

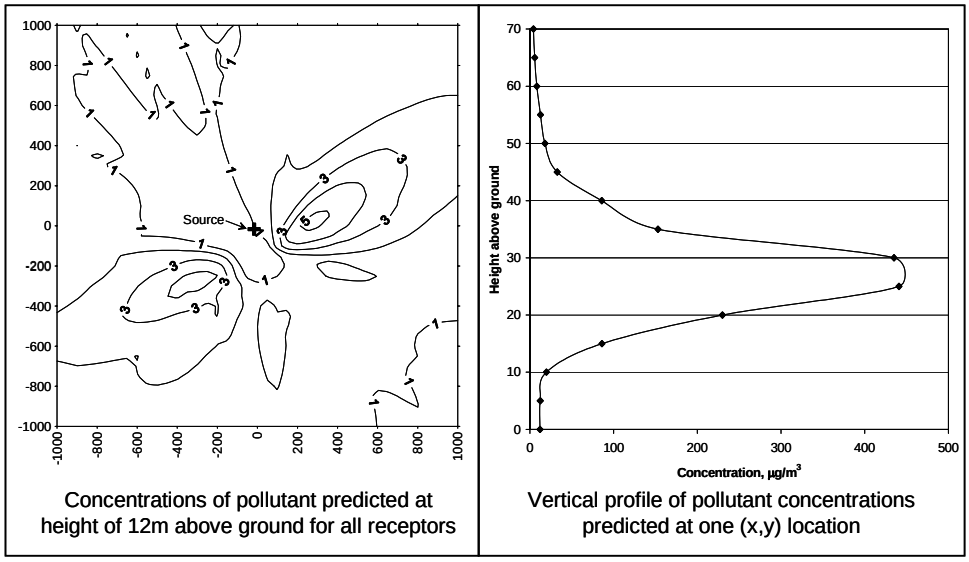
Flagpole receptors are available in AUSPLUME, ISCST3 and CALPUFF.

Recommendation 24

Use flagpole receptors when there is a requirement to calculate pollutant concentrations at some height above the ground.

An example of where you might use flagpole receptors is when you are modelling pollutant emissions in an area where there are tall buildings that have air conditioning intake ducts on their roofs, or where upper-storey windows may be opened for ventilation. The flagpole receptor option may also be used to look at changes in plume rise and vertical spread downwind from the source. Two examples of the use of flagpole receptors are shown in Figure 4.8.

Figure 4.8: Two examples of the use of flagpole receptors



Flagpole receptors should be distinguished from elevated receptors that are at ground level but at a higher elevation than the base of the source due to changes in terrain. Ground-level concentrations for the latter type of elevated source are calculated by a different method to those for flagpole receptors, so you should be careful to specify the nature of the elevation of your receptors in the correct way in the model.

4.2.4 Complex terrain

Changes in terrain around an air discharge source can significantly affect the pattern of dispersion of the discharge plume. Steady-state Gaussian models like AUSPLUME and ISCST3 contain simple algorithms to attempt to account for the effects of terrain in a limited fashion. CALPUFF contains much more sophisticated procedures for modelling the effects of terrain, with correspondingly greater effort required by the modeller to specify the terrain data.

TAPM handles complex terrain by using a terrain-following co-ordinate system and solving fundamental equations for wind, temperature, moisture, rain, turbulence and pollution dispersion. Using TAPM in complex terrain is relatively easy, as TAPM comes with an easy-to-use GUI that allows users to configure a simulation for any region using provided data sets of terrain, land use and synoptic-scale meteorology. User-defined data sets can also be provided to TAPM to allow more detailed local data to be used if available.

Because of the assumption that the wind speed and direction remain constant over the full length of the plume, Gaussian-plume models like AUSPLUME can only partially simulate terrain effects (VicEPA, 2000). Complex terrain may produce wind channelling around or between hills and ranges, especially under stable atmospheric conditions.

Recommendation 25

In complex terrain, Gaussian-plume models should only be used to provide a screening assessment and then only for impacts on terrain features that are adjacent to the source.

The limitations of Gaussian-plume models to accurately simulate dispersion in complex terrain must be acknowledged and accounted for in any assessment where terrain may influence dispersion, or where receptors are located on topographical features.

If terrain is potentially significant to a simulation then consider using CTDM, CTSCREEN or an advanced model. Justify the choice of model if a steady-state one is used.

However, if local terrain is not significant and a decision has been made to use AUSPLUME or ISCST3, sensitivity studies (NIWA, 1998) suggest that:

- terrain more than 10% of stack height and in the range 5–50 m should not be ignored
- for terrain heights smaller than 10% of stack heights a 10% underestimate in peak concentration is likely to occur.

a How does terrain affect plume dispersion?

Local topography can have several influences on plume transport and diffusion (Katestone Scientific, 1998):

- Upwind terrain can alter the wind flow and turbulence characteristics from those measured at the nearest meteorological station. Hills or rough terrain can change wind speeds, directions and turbulence characteristics, and nearby water bodies can considerably dampen turbulence levels.
- Significant valleys can restrict horizontal movement and dispersion and encourage the development and persistence of drainage flows. Night-time values of horizontal turbulence can be considerably reduced.
- Sloping terrain may help to provide katabatic or anabatic flows (i.e. drainage of air down or up hillsides in response to changing vertical temperature profiles).

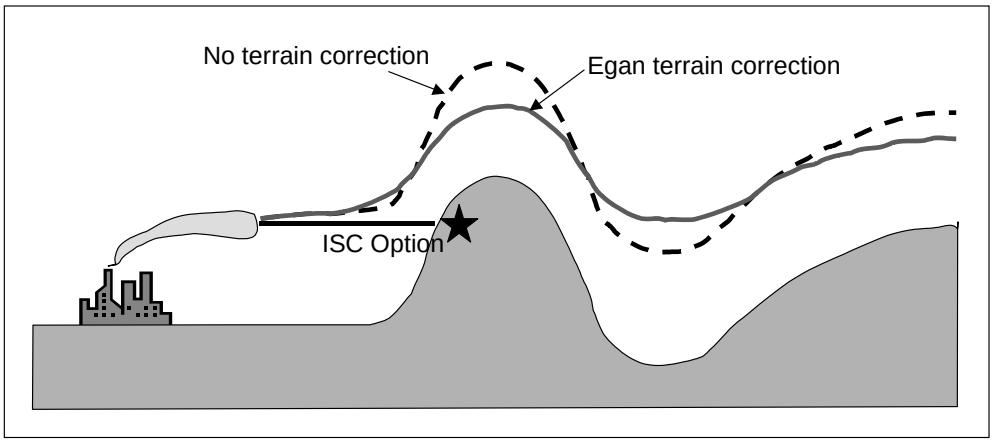
b How does AUSPLUME handle terrain?

AUSPLUME 5 offers three options for terrain adjustment calculations. These are outlined below, using the descriptions from the AUSPLUME online help system. The differences between these three options are shown in Figure 4.9.

- **ISC method (horizontal plume):** The simplest terrain correction assumes that the terrain has no influence on the plume height above sea level (i.e. the plume is assumed not to be uplifted at all by the terrain below it). Although called the 'ISC method' in the AUSPLUME help, the terrain approach used by the current version of ISCST3 is more complex than this, as described below in (c).

- **Egan half-height approach:** In neutral or unstable conditions, a plume will tend to be uplifted by broad terrain features. Under stable conditions, this lifting will generally be less and the plume will pass closer to the face of the hill and may even impact on the surface. On the other hand, plumes passing into a valley will tend to move further from the ground. In both situations the variation in plume centreline height above the local terrain becomes more apparent as atmospheric stability increases. These situations are simulated by allowing the plume axis to remain at the plume stabilisation height above mean sea level under stability categories E and F (stable). For unstable and neutral conditions (categories A to D) the half-height correction factor is used for changes in plume axis height above varying terrain (see Figure 4.9). The plume axis is constrained to be at least 10 m above ground level. This is the preferred terrain correction option.
- **Modified Egan approach:** The third option is simply a generalisation of the Egan method that allows the user to specify the constant of proportionality of approach for each of the six Pasquill stability classes. This option is only recommended where observational data exist to justify its use.

Figure 4.9: Options for simulation of terrain adjustments in AUSPLUME



Recommendation 26

When using AUSPLUME to assess the impact of discharges on elevated receptors, use the Egan half-height approach as the primary assessment approach.

If using steady-state plume models to assess the impacts of discharges on elevated receptors, present the results from both ISCST3 and modified Egan approaches to provide some indication of the potential uncertainty contained in the assessment.

c How does ISCST3 handle terrain?

Terrain below release height is referred to as simple terrain. Receptors located in simple terrain are modelled with the ISC option described above for AUSPLUME (section 4.3.4b).

ISCST3 incorporates the US EPA's COMPLEX1 screening model algorithms for use with complex terrain (some or all receptors above final plume rise height) and intermediate terrain (terrain located between the release height and the plume height). For receptors located on intermediate terrain, the model will select the higher impact from the simple and complex terrain algorithms on an hour-by-hour, source-by-source and receptor-by-receptor basis. The COMPLEX1 algorithm is based on the Egan half-height method for AUSPLUME (section 4.3.4b), where the plume height relative to the stack base is deflected upwards by an amount equal to half of the terrain height as it passes over complex terrain during unstable and neutral conditions (this is the same in AUSPLUME). The plume height is not deflected by the terrain under stable conditions (in AUSPLUME the plume height is deflected by 35% by the terrain under stable conditions in the default Egan half-height method (Earth Tech, 2001)). However, sector average is used to account for plume deflection around the hill. This approach is not used in AUSPLUME.

The complex terrain screening algorithms apply only to point source and volume source emissions – area source and open pit emission sources are excluded – and do not include building downwash effects.

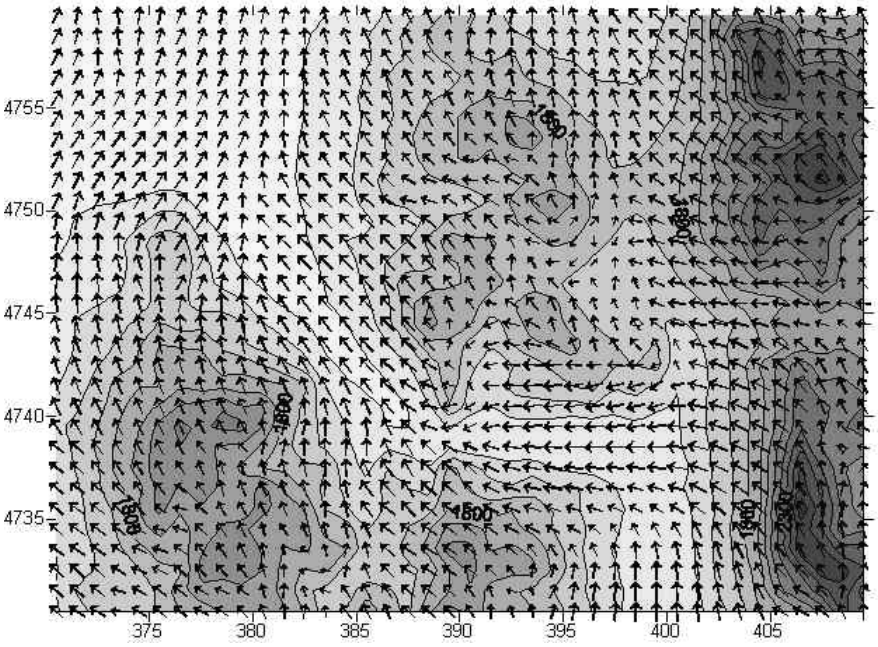
d How does CALPUFF handle terrain?

A considerably more sophisticated approach that permits the plume to flow both around and over terrain obstacles is used by CALPUFF. In the steep, complex terrain often encountered at sites in New Zealand, the use of CALPUFF is sometimes necessary. However the input and processing resources required to run this three-dimensional non-steady-state model are significantly greater than for either AUSPLUME or ISCST3. CALMET uses terrain and meteorological data to define a wind field for the modelling domain. Figure 4.10 shows an example of a wind field and illustrates how the wind vectors change to reflect the terrain.

CALPUFF then uses this wind field to model the dispersion and movement of the puffs. CALPUFF also uses the same Egan half-height method as AUSPLUME to model the movement of puffs over terrain. A more complicated option, the 'strain-based dispersion adjustment', is also offered. In addition, CALPUFF simulates the interaction of puffs within sub-grid-scale terrain. The sub-grid terrains feature is used when concentration estimates are required at locations on terrain elements not resolved by the grid in the flow-field model. It requires that the terrain feature being considered is identified and described within CALPUFF. Ideally, though, all important terrain features should be resolved by CALMET.

Users wanting more information on these options should refer to the CALPUFF user's guide.

Figure 4.10: Example of a wind field calculated by CALMET



Recommendation 27

Use an advanced model in an assessment which involves complex terrain only when either:

a) a good quality meteorological file is available; or

b) a good-quality meteorological file can be produced for the site in question.

e How accurate are results when terrain effects are significant?

The more complex the situation a model is required to simulate, the poorer its performance is likely to be. However, some models will handle complex terrain much more realistically than others.

Plume model results must be treated with due caution when terrain effects are significant. There are three inherent limitations with plume models in complex terrain:

- rudimentary treatment of terrain effects on plume lift
- no consideration of causal effects (i.e. the time it takes pollutants to travel to the terrain features), which means that only effects on terrain adjacent and close to the source should be considered
- the straight-line trajectory of the airflow.

Puff models are fundamentally different from plume models. Their non-steady-state nature allows them to account for causal effects and non-straight-line trajectories, so, in principal, puff models will produce more accurate results than plume models when terrain effects are significant. However, in a complex terrain situation, one should never assume an advanced model will overcome all potential problems. It may transpire that the specific issues of a situation determine that none of the available models will provide useful information.

A comparison between ISC3 and CALPUFF showed that in a steady-state environment results were similar (US EPA 1998b). However, in a variable state environment (i.e. complex terrain) there is a trend toward higher concentrations being simulated by CALPUFF. This trend is reversed when the terrain is at greater distances from the source.

4.2.5 Where can you get detailed digital topographical data?

If terrain data are required they can be read from a 1:50,000 scale topographical map for simple cases, although the resulting precision and digital reproduction will not be particularly accurate. A terrain reading will be required for every receptor on the grid, which can be a tedious task. If the terrain detail precision is important, and/or reading from a topographical map will be too time-consuming, then digitised terrain data for New Zealand can be purchased from several agencies such as Terralink International Ltd (http://www.terralink.co.nz/) or GeographX (NZ) Ltd (www.geographx.co.nz). Although the original terrain data are public data and free to all, these agencies charge a licence fee for providing the data in a useable format and for updating the data set.

Terralink International Ltd also provides a new database called the New Zealand Landcover Database, which contains both terrain and land-use data at 100 m resolution. The land-use data are necessary for modelling with CALPUFF.

These data sets are upgraded regularly, and are becoming increasingly easier to access.

Recommendation 28

Obtain and use terrain data with a resolution that will identify terrain features that are important for the problem under consideration.

4.3 Which buttons do I push?

There are many different ways to configure a model, and variations to the input parameters can have significant effects on a model's results. These include:

- dispersion parameter schemes (section 4.3.1)
- plume rise parameters (section 4.3.2)
- partial plume penetration (section 4.3.2)
- building wake effects (section 4.3.3)
- averaging times (section 4.3.4).

It is important to use the most accurate and appropriate parameters, both for your model and for the particular situation you are trying to simulate. It can be tempting to choose an option that gives you favourable results, without considering how sensitive your model is to that option.

Recommendation 29

Configure the model to reflect the reality of the situation as closely as possible.

Clearly describe and explain the options chosen in the method.

If unsure which option to use, or if several options could be applied, run the model using each option and present both the most conservative and the realistic set of results.

4.3.1 Dispersion coefficients

Dispersion coefficients are the horizontal and vertical dispersion parameters used to define the rate of dispersion of contaminants in the plume in the horizontal and vertical directions (i.e. plume width and height). In Gaussian-plume/puff models such as AUSPLUME, ISCST3 and CALPUFF, these coefficients are a function of atmospheric stability and distance from the source. In models that use more fundamental equations of atmospheric dispersion, such as TAPM, the dispersion is calculated internally by the model using the predicted meteorology and turbulence.

There are three types of horizontal dispersion coefficients available in AUSPLUME, ISCST3 and CALPUFF: Pasquill-Gifford (P-G), Briggs Rural (B-R), and the standard deviation of wind direction known as sigma-theta (σ_θ).

The P-G dispersion curves were developed from 10-minute average experimental data from near ground level, released in flat terrain. The B-R formula was derived from experiments on dispersion from tall stacks (of which there are very few in New Zealand).

For any model, hourly-averaged conditions can lead to over-prediction of concentrations, as the wind direction is assumed constant for each hour and pollutants arrive at the same location for the full period. If this causes pollutant levels of concern, the hour-by-hour meteorological conditions should be checked. If conditions are roughly constant for a number of hours, it is safe to assume that they are constant within each hour. Variations on sub-hour time scales should be parameterised through the horizontal dispersion coefficients (σ_θ). Higher variability implies a larger dispersion coefficient and a lower hour-averaged concentration, which is more realistic. Wherever possible, horizontal dispersion coefficients should be derived from observed wind-direction fluctuations, and this is generally included in plume models. Otherwise, the coefficients have to depend on the stability class.

Use of the σ_θ coefficient requires data on the standard deviation of wind direction to be included in the meteorological data file, although this will often not be available. Use σ_θ coefficients with caution. When highly stable conditions coincide with very low σ_θ values (i.e. very limited dispersion in both the horizontal and vertical directions), unrealistically high concentrations can be predicted. When using σ_θ coefficients it can be helpful to cross-check your results by rerunning the model using P-G dispersion curves and comparing results.

The P-G is the most commonly used dispersion coefficient scheme used in ISCST3 and is selected when rural conditions are modelled. However the urban option automatically uses the McElroy Pooler coefficients calculated from the Briggs formula. CALPUFF does the same if the default dispersion coefficients are selected. Note that when you choose the urban option in ISC3ST3 you get both the urban (McElroy-Pooler) dispersion coefficients and the urban wind profile.

Compared with the commonly used dispersion schemes, CALPUFF also has more sophisticated methods to calculate dispersion coefficients from meteorological variables. Scire et al. (2000a) provide a detailed description of the 'similarity theory' and 'real turbulence' dispersion schemes. These schemes are widely recognised as being more scientifically robust and are therefore a potentially better option for the modeller to use.

Recommendation 30

When using steady-state Gaussian-plume models, use:

a) Pasquill-Gifford dispersion curves for all sources except those with very tall stacks

b) Briggs-Rural dispersion curves for stacks higher than 100 m

c) the same type of vertical dispersion coefficient as selected for the horizontal equations

d) measured turbulence parameters (i.e. σ_θ) only when good-quality and appropriate meteorological data are available *and* when it can be demonstrated that using σ_θ produces superior results to using P-G or B-R schemes.

When using advanced models, consider the available turbulence/dispersion schemes, and use the option that:

a) makes best use of the available meteorological data (e.g. measured turbulence parameters)

b) is the most appropriate and useful scheme for the case under consideration – use a sensitivity analysis of the model's performance to the different turbulence/dispersion schemes to identify the most appropriate and useful option.

For more detailed information on the use of dispersion coefficients, refer to the user's guide for the particular model being used.

If you are using a steady-state Gaussian model, you should note the following guidelines for range applicability of Gaussian-plume models (CASANZ, 1998).

- The P-G curves used to define dispersion coefficients are applicable over distances up to about 1 km from the source.
- The P-G curves can also be extrapolated out to distances of about 10 km from the source but with a loss of accuracy due to changes in wind speed, direction, terrain and surface roughness, which would occur as the plume travels over that distance.
- The P-G curves are much less reliable for receptors less than about 100 m from the source.

Recommendation 31

The approximate range applicability of plume models is:

a) receptors < 50 m from source – acknowledge large uncertainties and do not rely on model results (applies to most models, but AERMOD, ADMS, then ISCPRIME and AUSPLUME-PRIME may perform better in this circumstance)

b) receptors 50 m – 100 m from source – use model results with some caution

c) receptors 100 m – 10 km from source – this is the usually accepted range of model applicability, although results for distances greater than about 5 km will lose accuracy due to wind shifts over that distance

d) receptors >10 km from source – do not rely on plume model results; instead use a mesoscale or regional model which uses wind fields over the extent of the grid.

Wind directional shear, surface roughness and the selection of rural or urban wind profile exponents also affect the rate at which the plume spreads and must be considered when modelling. These are discussed below.

a Wind direction shear

Any variation in wind direction over the plume depth (wind shear) will give rise to an effective lateral dispersion which becomes a significant additive effect on the horizontal spread of the plume at long distances downwind from the source (>10 km). Some models provide an option to estimate the enhancement in the lateral dispersion due to wind direction shear.

Recommendation 32

Adjustment for wind direction shear should only be used where there are receptors more than 10 km from the sources.

Before configuring the model to adjust for wind shear, check the model's manual to ensure that any other prerequisite criteria are met.

It is unlikely that the option in AUSPLUME or ISCST3 for 'adjustment for wind directional shear' will ever need to be used. However, in CALPUFF shearing of puffs is accounted for, and the use of wind direction shear is appropriate.

b Surface roughness

Topographic features, buildings or vegetation increase the ground's surface roughness. For all but the unstable categories (where convective turbulence dominates), surface roughness increases the vertical mixing of a plume and changes the wind-speed profile at elevated heights because of the enhanced mechanical turbulence generated as the air moves over the ground (VicEPA, 2000).

Both the height and spacing of roughness elements at the surface will influence the frictional effect on the wind. Typical values of surface roughness length are shown in Table 4.1.

Table 4.1: Surface roughness lengths for typical surfaces

Type of surface	Surface roughness length (m)
Urban	1.0–3.0
Coniferous forest	1.3
Cultivated land (summer)	0.2
Cultivated land (winter)	0.1
Grassland (summer)	0.1
Grassland (winter)	0.001
Water	0.0001

Source: Schnelle and Dey, 1999

AUSPLUME uses a simplified range of land-use categories and their approximate surface roughness heights for dispersion calculations (see Table 4.2), although other surface roughness heights can also be used. The type of land use both upwind and downwind of the source should be considered when choosing a land-use category, as both will affect the wind-speed profile. In situations where a range of land-use types must be considered, the modeller may choose to:

- use the category that has the lower surface roughness value, which will produce a more conservative ground-level concentration
- estimate an average surface roughness value for the area and choose the land-use category that is closest to this value.

The AUSPLUME user's guide (VicEPA, 2000) notes that reported values of the surface roughness height vary greatly even for the same nominal land use, and that the surface roughness heights entered into the model when you select a land-use category should be a general guide only.

Table 4.2: Land-use categories and surface roughness length in AUSPLUME

Land-use category	Surface roughness length (m)
Hills	2.0
High rise	1.0
Industrial	0.8
Commercial	0.8
Residential	0.4
Forest	0.8
Rolling rural	0.4
Flat rural	0.1
Flat desert	0.01
Water	0.0001

Figure 4.11: Effect of surface roughness height on dispersion from a volume source using AUSPLUME

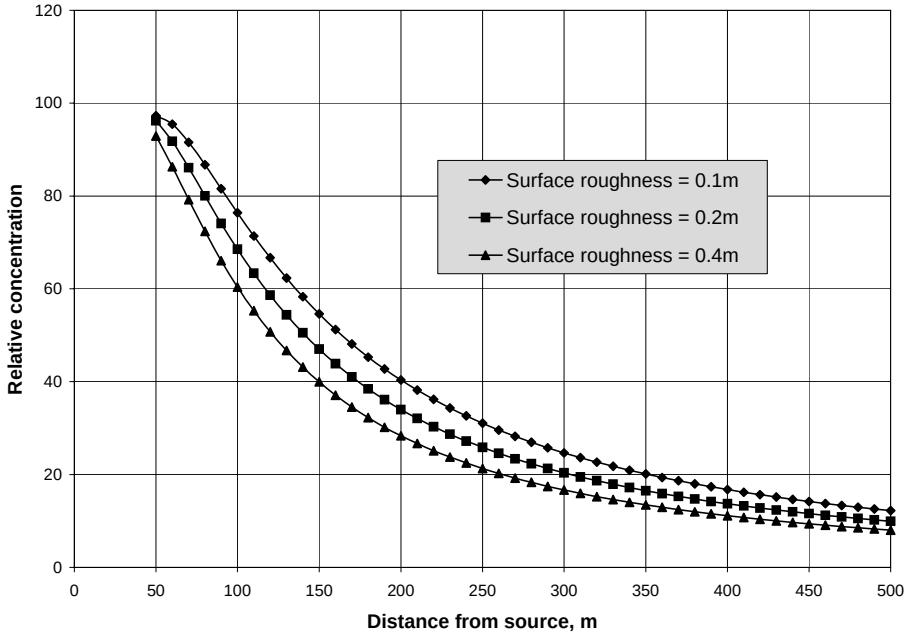


Figure 4.11 is an example (using AUSPLUME) of a sensitivity analysis for surface roughness. This suggests that the relative effect of changing surface roughness increases with distance from the source. The effect of surface roughness will vary depending on the type of source being modelled. Surface or near-surface releases tend to show a greater sensitivity to changes in surface roughness than do releases from tall stacks.

ISCST3 and ISC-PRIME do not incorporate surface roughness into their dispersion calculations but offer a choice of either urban or rural land use to account for the effect of land use on dispersion characteristics. CALPUFF incorporates the effect of surface roughness via land-use data used at the CALMET meteorological pre-processing stage.

Recommendation 33

When assigning a surface roughness to the domain being modelled, attempt to capture characteristics representative of the area in which the maximum concentrations are likely to occur (i.e. within 200 m of a surface or near-surface release and up to 10 km for tall stacks).

When choosing a surface roughness length, consider the sensitivity of the model's output to the value of the factor chosen.

Select the smallest relevant surface roughness factor for the area being studied.

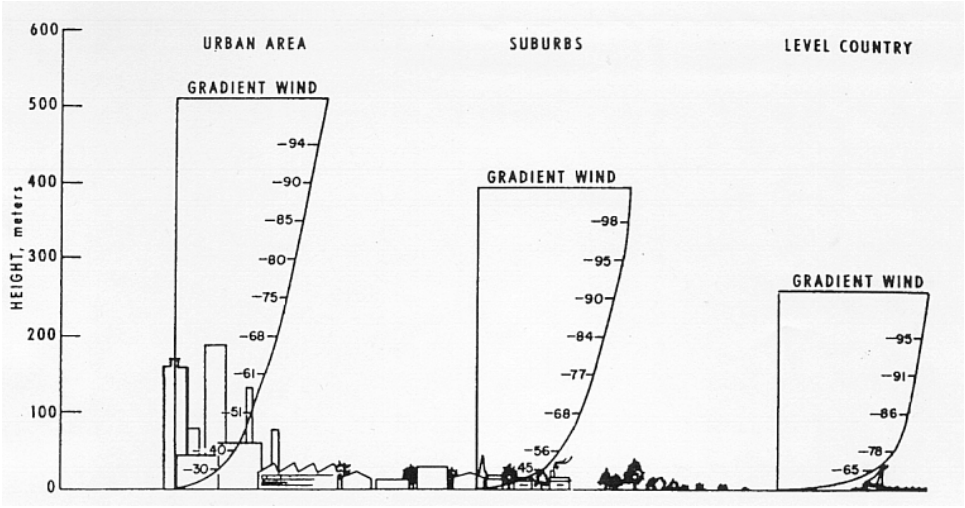
The use of the most relevant surface roughness height will not always give the highest concentration. For example, from an elevated emission, particularly close to the source, the increased vertical dispersion resulting will bring the plume down to ground sooner for larger surface roughness heights.

c Wind profile exponents (rural versus urban)

To calculate plume rise, the wind speed at the stack height is estimated by extrapolating from the wind speed measured by the anemometer (often located at a standard height of 10 metres) (VicEPA, 2000). The extrapolation calculation uses a power law equation with a wind profile exponent. Wind profile exponents are most strongly influenced by surface roughness and are a function of the Pasquill stability category.

Wind profile exponents can be specified as rural or urban. The dispersive characteristics of the atmosphere are different over large urban areas, which might have significant surface fractions of concrete, roads and buildings (Figure 4.12). In some circumstances, the choice of urban or rural dispersion curves can make a substantial difference to the maximum ground-level concentration predicted. Results using urban values are typically one to five times higher due to additional convection caused by urban surfaces, although the reverse can be true for ground-level area sources.

Figure 4.12: The effect of surface roughness on wind speed



Source: Schnelle and Dey, 2000

The models' users guides contain guidance for determining whether the surrounding land should be classified as rural or urban.

Recommendation 34

Using height and density of building development as criteria, classify the land use for the area contained within a 3 km radius (approximately) from the source. If more than 50% of this area is urban (i.e. reasonably high density of buildings), then urban dispersion coefficients should be used, otherwise rural coefficients should be used.

Where the surrounding area may have an equal mix of both urban and rural land use, run the model using both options and present the range of results. The actual effects are likely to be somewhere between the two.

Bodies of water are not included in this calculation (Trinity Consultants, 1996). It is generally considered that the majority of New Zealand cases will be classified as rural, because urban development tends not to be as heavily built up as in many overseas examples (NIWA, 1998).

4.3.2 Plume rise

The height of the plume centreline at some downwind distance is the sum of the initial discharge height, the plume rise due to buoyancy and the plume rise due to the initial momentum of the discharge, minus the stack-tip down-wash (VicEPA, 2000). In addition to the effects of building wakes on plume rise described in section 4.3.3, there are three types of plume rise options that can be selected:

a) gradual rise of a buoyant plume

b) partial penetration of elevated inversions

c) plume downwash from behind a stack (stack-tip downwash).

In AUSPLUME you must select either option (a) or (b), because the model will not calculate both at the same time. It may be necessary to run the model with first one and then the other option selected to see which option creates the greatest ground-level concentration. Option (b) is not available in ISCST3. In CALPUFF, both options (a) and (b) can be simulated together.

In 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. TAPM calculates plume rise using predicted 3-D meteorology and turbulence. Gradual plume rise and stack-tip downwash are automatically used in LPM mode, while only stack-tip downwash is used in EGM mode. TAPM developers recommend that when using TAPM, significant point sources should be run in LPM mode wherever possible/practical when near-source maximum concentrations need to be modelled accurately.

a Gradual plume rise

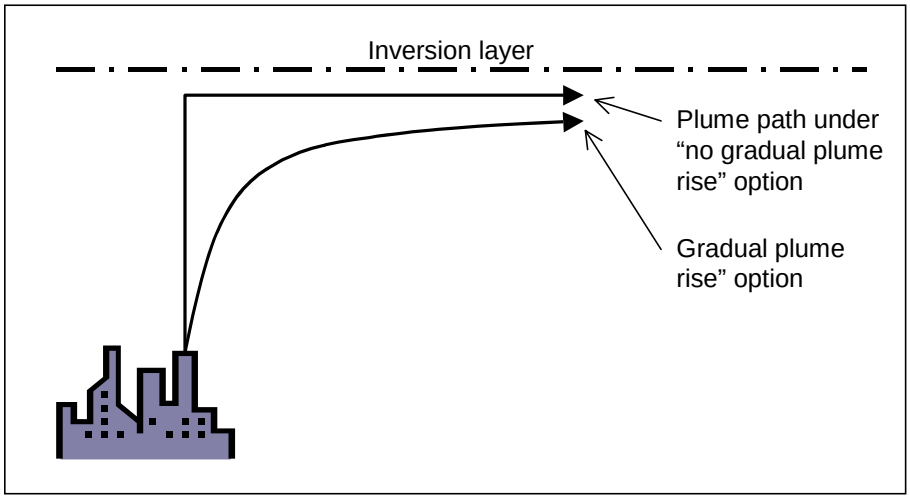
When gradual plume rise is selected, the plume rises gradually to its final height as it travels downwind (Figure 4.13). The gradual plume rise mechanism is physically realistic but mathematically simplistic. If this option is not selected, the model assumes the plume is at the final plume height everywhere when calculating ground-level concentrations, rather than calculating plume height as a function of downwind distance. If the partial penetration of plumes through an elevated inversion layer (option b) is required, then in AUSPLUME the gradual plume rise option cannot be selected. This is likely only in cases of tall stacks whose plumes quickly rise towards the inversion height; otherwise it is physically unrealistic to not select the gradual plume rise option.

Recommendation 35

In AUSPLUME, select the gradual plume rise option unless there are tall buoyant sources and low mixing heights.

In ISCST3 the 'regulatory default' combination of dispersion and plume rise parameters include no gradual plume rise, so if the gradual plume rise option is required the regulatory default settings will need to be overridden (US EPA, 1995).

Figure 4.13: Gradual plume rise



b Partial penetration of inversions

An inversion layer can be described as thermal stratification between layers of the atmosphere that provides a resistance to vertical movement of the plume. If the plume has enough energy from its initial thermal buoyancy or vertical momentum to penetrate the inversion layer, some or all of the plume may become trapped above the layer and be unable to return to ground. Some Gaussian-plume models assume that plumes in the mixed layer below the inversion cannot penetrate upwards through the inversion base. However, observations show that in some cases the plume may penetrate the inversion layer. Partial penetration is shown in Figure 4.14.

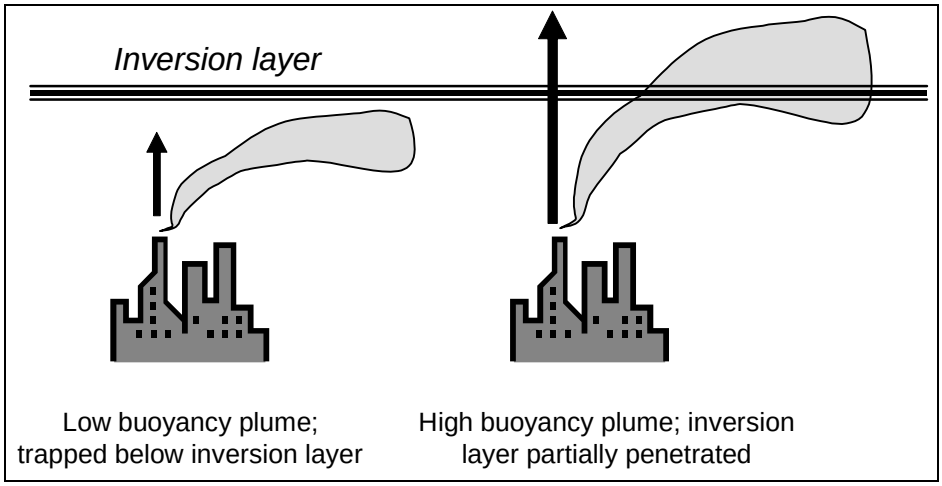
AUSPLUME, CALPUFF, CTDMPLUS and AERMOD provide an option for simulating the partial penetration of buoyant plumes through an elevated inversion. Partial penetration of elevated inversions is automatically handled by TAPM using the predicted 3-D meteorology and turbulence. For any simulated hour, concentrations will either increase if the plume penetrates downwards through the inversion base, or decrease whenever material is lost upwards from the mixed layer below. The AUSPLUME user's guide (VicEPA, 2000) notes that this option assumes that the plume reaches its maximum height instantaneously as it leaves the stack. Sacrificing the ability to model the gradual rise of the plume as a function of the downwind distance is only warranted for tall, buoyant sources such as power stations and smelters, because partial penetration of inversions is important in these cases and some models cannot simulate both partial penetration and gradual plume rise. Neglecting the gradual plume rise will underestimate concentrations wherever building downwash or impacts on nearby hillsides are important.

If the partial plume penetration option is selected, plume rise and emission rates are modified only if the:

- plume is buoyant
- plume height is within a certain range
- atmospheric conditions are unstable or neutral
- the simulated hour is between 6 am and 8 pm (i.e. during daytime).

For more information on how AUSPLUME calculates partial penetration, refer to the model's user guide.

Figure 4.14: Schematic of the interaction between plumes of different buoyancy and an inversion layer



Recommendation 36

Use the partial penetration option with caution, and only when there are tall buoyant sources and low mixing heights.

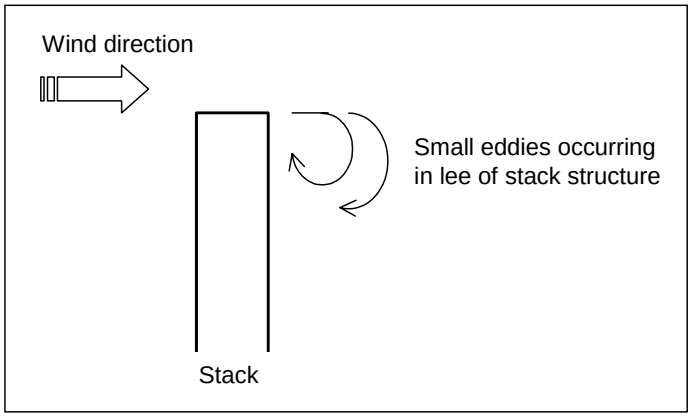
Describe the influence of partial penetration on modelling results by rerunning the model and comparing the results with this option switched off.

c Stack-tip downwash

This option allows for the downwash effects of chimney wakes; i.e. the downwind turbulence created by the stack itself (Figure 4.15). The amount of stack-tip downwash depends on the stack height and diameter, exit velocity and wind speed (VicEPA, 2000). A maximum reduction of plume rise of three stack diameters occurs when the exit velocity is zero. Since the reduction in plume height is never more than three chimney diameters, stack-tip downwash usually makes little difference to the results except for the receptors close to the stack.

Stack-tip downwash is also included in the regulatory default options in ISCST3. An exception may be large, stumpy stacks like tunnel vents, in which case you may want to consider turning stack-tip downwash off.

Figure 4.15: Example of stack-tip downwash



Recommendation 37

Select the stack-tip downwash option unless there is a specific reason not to do so.

4.3.3 Building downwash effects

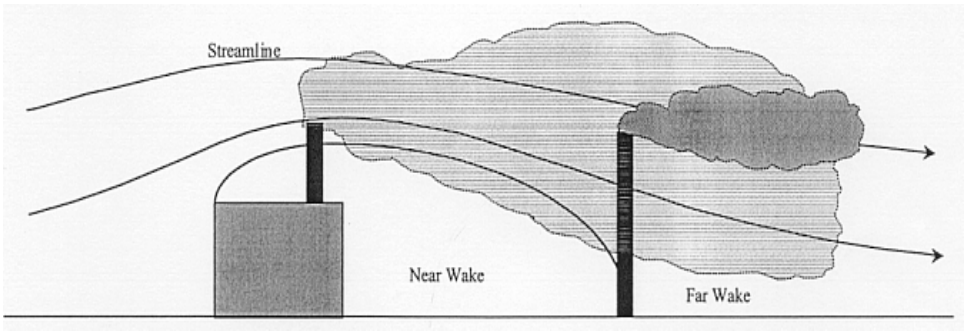
Airflow around buildings is often very complicated and may create zones of strong turbulence and downward mixing on the lee side of a building (Figure 4.16). This effect is known as building downwash. In such cases, the entrainment of exhaust gases released by short stacks or rooftop vents in the wake of a building can result in much higher ground-level concentrations close to the source than the model would otherwise predict. A well-designed stack can minimise building downwash effects. It is generally accepted that if a stack complies with the criteria in the Good Engineering Practice (i.e. 2.5 times higher than any nearby building), then building downwash is unlikely to occur (US EPA, 1985).

Much research has concentrated on ways to simulate building downwash. As a result, there are four main types of building downwash algorithms now in use:

- Huber-Snyder (H-S)
- Schulman-Scire (S-S)
- hybrid scheme (a combination of H-S and S-S)
- Plume Rise Model Enhancements (PRIME).

These algorithms are described in VicEPA (2000). In AUSPLUME, ISCST3, AERMOD, CALPUFF and TAPM building downwash effects are computed only for point sources.

Figure 4.16: Schematic of building downwash for two identical plumes emitted at different locations



Source: Schulman et al., 2000

The recently available PRIME algorithm has been proven to be superior to the H-S and S-S algorithms in verification studies (Paine and Lew, 1997). The PRIME algorithm is the default algorithm in AUSPLUME v5.4, although other algorithms can be selected by the user. The US EPA has modified ISCST3 to allow use of the PRIME algorithm, resulting in a new model called ISC-PRIME, which is now becoming the preferred model instead of ISCST3 in the United States. CALPUFF v6 and AERMOD also contain the PRIME algorithm. TAPM uses an approach based on the PRIME algorithm for point sources in LPM mode. The PRIME algorithm requires more detailed building dimension information than the H-S and S-S algorithms.

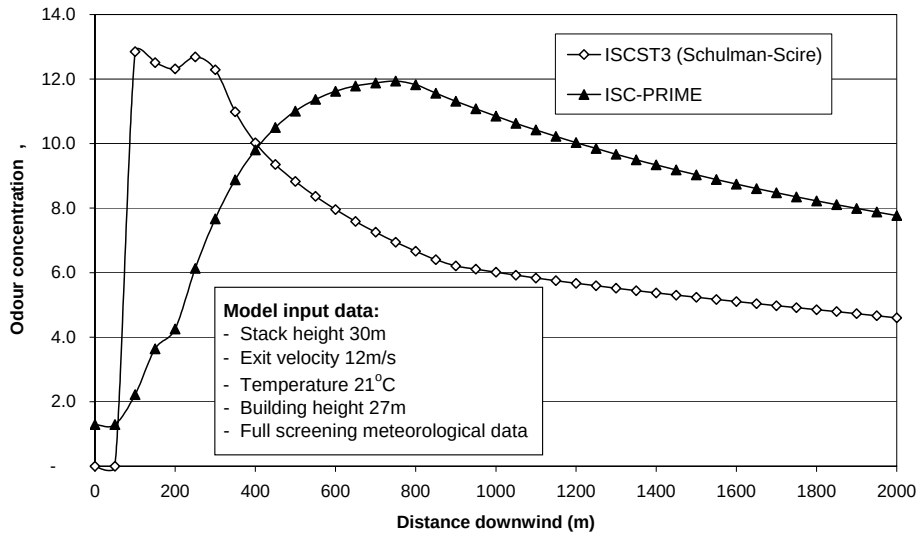
A full description of PRIME's treatment of plume rise and building downwash is given by Schulman et al. (1997 and 2000). It is recommended that modellers who intend using the PRIME algorithm make themselves familiar with the technical issues associated with this model's development and use.

In AUSPLUME (pre version 5) and CALPUFF (pre version 6) the user may choose one of H-S, S-S or the hybrid approach. One problem with the H-S algorithm is that it tends to overestimate ground-level concentrations in stable, low wind speed conditions (Thistle et al., 1995). If PRIME is not available, the S-S algorithm is recommended over either the H-S algorithm and the hybrid approach. ISCST3 uses the hybrid option by default, and the user cannot change this. A more productive option to take is to upgrade your model to a PRIME compatible version, rather than attempting to use any of the S-S , H-S or hybrid algorithms.

Figure 4.17 shows an example of the effect of selecting S-S or PRIME algorithms on model results where downwash is important.

Building dimensions for ISCST3, AUSPLUME, AERMOD and CALPUFF can be generated either manually or via the Building Profile Input Programme (BPIP), which is available free from http://www.epa.gov/ttn/scram/. With BPIP, the location and height of all buildings and stacks are entered and the subroutine calculates the direction-specific building dimensions. If the PRIME algorithm is being used, a modification to BPIP called BPIPPRM must be used, as special building dimension data are required. BPIP and BPIPPRM are easy to use, and the process is made even simpler by AUSPLUME v5, which has integrated BPIP and BPIPPRM into its graphical user interface (GUI). Some proprietary GUIs for ISCST3, such as those of Trinity Consultants or Lakes Environmental (1996), also include the BPIP subroutine in their GUI.

Figure 4.17: Example of the effect of selecting a building wake algorithm on dispersion



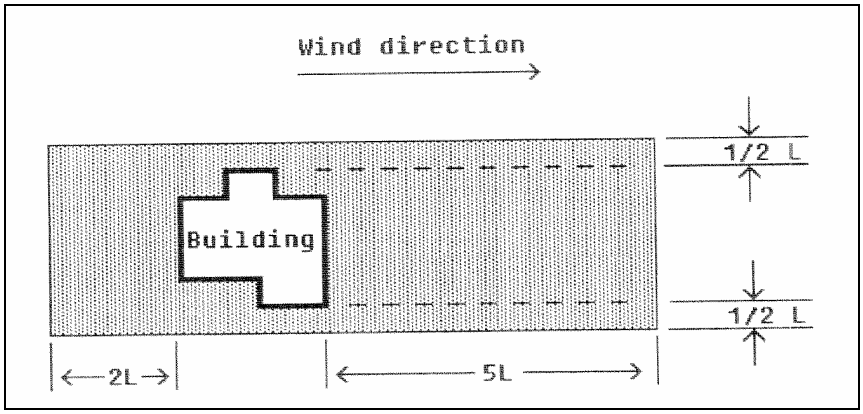
The output from BPIP and BPIPPRM includes building height and width information for wind directions at 10 degree intervals. Note that although there is a difference in wind direction convention for the input meteorological data between AUSPLUME and ISCST3, both models correctly use the BPIP/BPIPPRM output.

TAPM doesn't use the BPIP-based approach (described above) for treating multiple buildings. The effects of overlapping wakes from multiple building blocks, whether from the same multi-level or multi-tiered physical building, or from multiple physical buildings, are treated by combining the meteorology and turbulence from overlapping wakes. Plume rise is affected by the modified meteorology and turbulence for point sources in both EGM and LPM modes, while dispersion is influenced only for point source plumes in LPM mode. LPM calculations in the model are done for both the cavity and wake regions, rather than specifying a uniform concentration in the cavity as is done in PRIME.

In initially assessing whether building wake effects are likely, a building should be considered sufficiently close to a stack to cause wake effects if the distance between the stack and the nearest part of the building is less than or equal to five times the lesser of the height or the projected width of the building. For downwash analyses with direction-specific building dimensions, wake effects are assumed to occur if the stack is within a rectangle comprising two lines perpendicular to the wind direction, one at 5 L downwind of the building and the other at 2 L upwind of the building, and by two lines parallel to the wind direction, which are each 0.5 L away from the side of the building, as shown in Figure 4.18.

If building wake effects are likely, the algorithms discussed above permit a simple treatment of the effect on ground-level concentrations. However, conventional diffusion approaches employed in such models can be misleading in complex flow situations. Consequently, where significant interactions between several flow obstacles are likely, and model predictions within the downwash area are critical, recourse to either wind-tunnel simulations or computational fluid dynamics (CFD) models may be necessary (e.g. Georakis et al., 1995).

Figure 4.18: Region of wake effect in direction-specific building downwash calculations



Note: L is the lesser of the height and projected width.

When using AUSPLUME-PRIME, careful note should be taken of the conditions under which the validation studies (Paine and Lew, 1997) of ISC3-PRIME were undertaken. AUSPLUME-PRIME may not default to the same dispersion curve scheme as used in the validation of ISC3-PRIME. This difference may affect the validity of AUSPLUME-PRIME results.

Building downwash effects are more likely to occur and will be most strongly observed during periods of relatively high wind speeds, so it is important that the meteorological conditions during which the maximum concentrations are predicted are considered when assessing the potential effects of building downwash. If maximum concentrations occur at very low wind speeds and at some distance from the building, it is unlikely that they are due to building downwash effects. Conversely, if the maximum concentrations occur close to the building when wind speeds are high, it is likely that building downwash effects are occurring. This may be checked by re-running the model with the building downwash algorithm switched off.

Note that there is a trade-off when using the building wake algorithms in AUSPLUME and ISCST3. When the building downwash algorithm is switched on, the gradual plume rise, stack tip downwash and ISCST3 COMPLEX1 algorithms are negated.

Recommendation 38

Assess whether building wake effects influence the results by running the dispersion model with and without building wake effects.

Use the PRIME building downwash algorithm if available. Consider upgrading your model if it does not contain the PRIME algorithm.

Use the most conservative of the S-S, H-S or hybrid algorithms if PRIME is not available.

When reporting building wake results, acknowledge the complex nature of plume/building interactions and the increased uncertainty contained in calculations of results within zones affected by building wakes.

Carefully consider the additional uncertainty in ground-level concentrations predicted for receptors within the near wake (i.e. within three building heights or widths).

If model predictions among buildings and in the downwash area are critical, then a computational fluid dynamics model should be considered.

4.3.4 Averaging times

a Averaging periods available

Most dispersion models permit ground-level concentrations to be calculated for a range of averaging times. The minimum averaging time for ISCST3 and CALPUFF is one hour, because the meteorological data are treated as hourly averages. Future versions of CALPUFF may allow meteorological data to be simulated at shorter intervals, and the minimum averaging time will also be reduced.

TAPM uses a numerical time-step of five minutes, and outputs hourly averaged meteorology and pollution concentration. Post-processing options are currently available to generate longer averaging times for pollution concentration, while post-processed pollution concentration for averaging times shorter than one hour are planned for a future version of TAPM.

AUSPLUME also uses one-hour meteorological data but allows the calculation of concentrations for averaging periods of less than an hour. The minimum averaging time that AUSPLUME will allow is three minutes.

To calculate concentrations for periods of less than one hour AUSPLUME undertakes a three-step process. Firstly, AUSPLUME modifies the original three-minute average sigma-y curves for a 60-minute averaging period. The aim of this process is "to represent the various factors involved in the dispersion process as realistically as possible" (Victoria EPA, 1985, p. 40), and it is designed to allow for increased dispersion due to wind meander during averaging times longer than three minutes. The difference between the three-minute and 60-minute sets of sigma-y P-G curves is determined by the approach recommended by Hanna et al. (1977). The following equation represents this relationship:

$$\sigma_{y\,60\,\mathrm{min}} = \sigma_{y\,3\,\mathrm{min}} \left[\frac{60}{3} \right]^{0.2}$$

This approach gives a ratio of 1.8 between the three-minute and 60-minute sigma-y dispersion curves.

Secondly the 60-minute sigma-y curves are scaled for the desired shorter time period (T) using the power law equation below:

$$\sigma_{y(T\,\mathrm{min})} = \sigma_{y(60\,\mathrm{min})} \left[\frac{T}{60} \right]^{0.2}$$

Thirdly, the concentration for the time period T is calculated by AUSPLUME using the modified sigma-y ($\sigma_{y\ T\mathrm{min}}$) produced in step 2. Some modellers manually convert one-hour average concentrations to shorter time periods by using a power law equation. The formula most frequently used is:

$$C_t = C_{60} \left[\frac{60}{t} \right]^x$$

where C_{60} = concentration for one-hour average
t = averaging time, in minutes
C_t = concentration for time of t minutes
X = is a coefficient ranging from 0.17 to 0.6.

This manual conversion will produce similar results to the modifying sigma-y approach undertaken in AUSPLUME. The exponent X in this power law equation is often quoted as being 0.2. Using this equation, the correction factors for various averaging times and where x = 0.2, are as follows:

Table 4.3: Correction factors for various averaging times

Averaging time, *t* (minutes)	Factor by which to multiply one-hour concentration (C_{60}) to get concentration for time of t minutes
3	1.82
10	1.43
30	1.15

The best value of X to use depends largely on the degree to which the site experiences convection, and can range from less than 0.2 for tall stacks in a highly convective situation, to as much as 0.6 for low-level releases in stable atmospheres.

However, recent research has shown this formula to be too simplistic and that its use cannot be justified (Venkatram, 2002). For most situations it can lead to a severe under-estimation of maximum short-term concentrations (Katestone Scientific, 1998). This is most likely to be a problem for odour simulations, and is discussed in more detail in the Ministry's revised *Odour Management Guide* and supporting documents (Ministry for the Environment, 2001).

This formula should not be used to estimate concentrations for longer averaging times than one-hour averages (e.g. using screening meteorology to get the maximum one-hour average, and then estimate 24-hour or annual averages from the exponential relationship). The longer-term averages are determined by meteorological patterns for the particular location, which will not be represented by the exponential relationship. For example, maximum one-hour average concentrations may occur in different wind directions from maximum 24-hour or annual average concentrations because prevailing wind directions do not necessarily give maximum short-term concentrations.

Averaging times for pollutants in the Ministry's *Ambient Air Quality Guidelines*, as proposed in the 2001 review, require a minimum time of one hour, plus other times of eight hours, 24 hours, three months, and annual (Ministry for the Environment, 2001). These averaging times can all be computed by AUSPLUME, ISCST3 and CALPUFF, but the accuracy of the results is determined by the quality of the meteorological data used.

Recommendation 39

Configure the model to calculate concentrations for an averaging period that is consistent with the assessment criteria being used.

Calculate results only for averaging times that are equal to or longer than the time-step of the meteorological data set being used.

The use of the relationship that calculates average concentrations for periods shorter than one hour should be avoided. If this relationship is employed, its suitability for that task must be justified, especially the choice of the exponent X (refer equations in section 4.3.4).

Do not calculate average concentrations for periods longer than 1 hour if using screening meteorological data.

b AUSPLUME versus ISCST3 one-hour averages

AUSPLUME and ISCST3 calculate one-hour average concentrations using the dispersion equations that are principally the same. But if you compare one-hour average results for AUSPLUME and ISCST3 (which are configured for an identical source), the ISCST3 results will be higher by a factor of approximately 1.8. This difference is primarily a result of the dissimilar manner in which the two models treat the Pasquill-Gifford horizontal (sigma-y) dispersion curves. This different manner in which AUSPLUME and ISCST3 treat sigma-y dispersion curves is described in section 4.3.4(a).

However if the results of an AUSPLUME and ISCST3 (configured for an identical source) are compared, it is unlikely the theoretical ratio of 1.8 that should exist between the two sets of results will actually be observed. Other differences between the two models that contribute to any deviation from the theoretical ratio of 1.8 include the following.

- ISCST3 defaults to McElroy-Pooler dispersion curves when in urban mode (this option is not available in AUSPLUME).
- P-G curves are adjusted for surface roughness in AUSPLUME (this adjustment does not occur in ISCST3).
- The vertical wind profile exponents do not match. AUSPLUME defaults to either Irwin urban or rural exponents. ISCST3 defaults to its own scheme.
- Wind speeds of less than 1 m/s are treated differently by the two models (section 4.5.5(a)).

To get AUSPLUME and ISCST3 results to agree as closely as possible you would configure:

- AUSPLUME to use ISCST wind profile exponents, P-G dispersion curves, surface roughness length of 0.03 metres for both the modelling domain and the meteorological site and a three-minute averaging time
- ISCST to use the rural dispersion scheme
- the meteorological data set so all wind speeds of less than 1 m/s are equal to 1 m/s.

Recommendation 40

ISCST3 should be acknowledged as likely to produce more conservative one-hour average concentrations than AUSPLUME (assuming both models are configured appropriately).

c Fixed versus moving averaging times

There are two approaches to calculating time-averaged concentrations: fixed averages, and moving averages. To illustrate the difference between these, consider an eight-hour averaging period. A fixed eight-hour average is reported three times per day, being the average of hours 01 to 08, 09 to 16, and 17 to 24. In comparison, a moving average would be reported 24 times per day, being the average of hours 01 to 08, 02 to 09, 03 to 10, and so on.

The *Good Practice Guide for Air Quality Monitoring and Data Management* (Ministry for the Environment, 2000b) recommends that both fixed and moving averages should be used for examining human health and environmental effects.

Most averaging times computed and reported by models are fixed, so if an assessment requires a moving average the model output will require post-modelling data processing. This can be achieved by importing the hourly model output data for a particular receptor into a spreadsheet where moving averages can be calculated and plotted from fixed one-hourly data.

Post-processing results (from models that do not include a moving-averages option) can become unwieldy if moving averages are calculated for all receptors. A practical approach to this problem is to identify the areas of highest impact from one-hour average concentration contour plots. For a small number of high impact receptors obtain all hourly values in the time period being modelled from an additional modelling run. Then post-process these results to analyse the moving average concentration.

Recommendation 41

Report both fixed and moving averages when assessing potential human health and environmental effects.

The type of average being used (i.e. fixed or moving) and the method used to calculate these should be clearly stated in the modelling methodology and reported with the model's results.

The averaging times computed in AUSPLUME 5 are:

- minutes – any number of minutes between 3 and 60
- hours – 1, 2, 3, 4, 6, 8, 12, 24 hours (fixed average)
- days – 90 days computed as a daily moving average
- months – three months, computed as a moving three-monthly average
- long term – averaged over the full meteorological data period.

Additional running averages for a number of percentile levels can be obtained by generating an AUSPLUME binary output file. The additional statistical information for averaging times between one hour and 24 hours can be obtained by running the statistics utility from the main menu (VicEPA, 2000).

The averaging times computed in ISCST3 are as follows: 1, 2, 3, 4, 6, 8, 12, or 24 hours, monthly averages (for calendar months), the average for the entire data period, and the annual average. The type of average (i.e. fixed or moving) is not specified in the user guides (US EPA, 1995 and US EPA, 1995b), but should be taken to be fixed averages.

Averaging times from CALPUFF runs are computed by the post-processor CALPOST. Averaging times of 1, 3, 24 hours, or length-of-run, are preset, or the user can specify any other averaging time of 1 hour or greater. The type of average (fixed or moving) is not specified in the user guide (Earth Tech, 2001), but should be taken to be fixed averages.

TAPM can produce either fixed or running averages for averaging times greater than one hour.

d Modelled versus measured medium-term averages

Fixed 24-hour averages in AUSPLUME, ISCST3 and CALPUFF are calculated from midnight to midnight (i.e. hour 01 to hour 24). If you are adding measured 24-hour average background data to these modelled results, be aware that the background data may be calculated on a different basis to the modelled data (e.g. 9 am to 9 am as used by Environment Canterbury). In many cases, this may not make a significant difference unless the meteorological conditions in the two data sets are significantly different from a dispersion perspective. These differences may also apply to other averaging periods.

4.3.5 Wet and dry deposition

When pollutants are emitted from a source, they disperse vertically in the turbulent air. Particles also settle towards the ground under the influence of gravity. Depending on the characteristics of the surface, pollutants may be removed from the air and deposited at the surface. Most models allow for the influence of gravitational particle settling on ground-level concentrations, with the user entering particle size distribution and density data into the model.

In addition, AUSPLUME 5, ISCST3, CALPUFF and TAPM can simulate the deposition of particles to the surface due to both:

- dry deposition (when the deposition is due to gravitational settling, turbulence and the nature of the ground surface)
- wet deposition (when the deposition is due to removal from the air by rain).

Dry deposition leads to a steady removal of pollutants from the air, in all weather conditions. However, precipitation can remove contaminants far more rapidly, cleaning the atmosphere in a single rain event.

Dry or wet deposition can be important whenever the source discharges significant amounts of large particles or certain other contaminants (e.g. metals and dioxins), which can occur from many source types. AUSPLUME 4 and earlier versions can calculate dry deposition only using a cruder methodology (VicEPA, 2000).

AUSPLUME 5, ISCST3, CALPUFF and TAPM also calculate plume depletion, due to either dry or wet processes, and material is removed from the plume as it is deposited on the surface.

Particle information (size, distribution and density) must be specified by the user if either dry particle deposition or depletion is requested. Particle size distributions (usually given in terms of aerodynamic diameters) have major effects on deposition rates. It can be a resource intensive exercise to obtain realistic and representative particle size distributions. Scavenging coefficients must be provided if either wet deposition or depletion needs to be modelled.

Wet deposition or depletion options will also require precipitation data to be available in the meteorological data file. In addition to rainfall in the meteorological data set, ISC requires friction velocity, Monin Obukhov length, surface roughness length and precipitation code. Therefore there is substantial work in developing a conventional ISC meteorological dataset to allow wet and dry deposition calculations to be made. AUSPLUME 5 will estimate friction velocity and Monin Obukhov length (although no information is given as to how it actually does this), so dry deposition can be computed without extra met file manipulation.

Gas deposition relates to surface adsorption of gases by vegetation. The ISCST3 and CALPUFF models also include algorithms to handle the scavenging and removal by dry or wet deposition of gases such as sulphur dioxide, sulphate, nitrate, nitrous oxides, and nitric acid. Gas deposition modelling is not commonly undertaken and will be most applicable only for large-scale discharges. Scavenging coefficients and special meteorological data must be specified by the user. For more information, refer to the models' user guides.

TAPM chemistry-mode includes dry and wet deposition processes for a number of species.

Recommendation 42

If modelling the effects of wet or dry deposition, demonstrate that good-quality input data are put into the model (such as deposition rates and specialised meteorological information).

In the near field (i.e. less than 10 km) and for (relatively) simple issues AUSPLUME and ISCST3 can be used to provide an indicative assessment of the effects of deposition.

In large modelling domains and for less simple issues, an advanced model which is designed to assess the effects of deposition should be used.

4.3.6 Atmospheric chemistry

Some pollutants are chemically reactive in the atmosphere. These include two types of pollutants.

- Pollutants that are unstable when discharged, and continue to dissociate into other chemicals as they disperse and are carried downwind – the effects of such reactions on ground-level concentrations may be significant over short ranges downwind if the reactions are fast.
- Gases such as nitric oxide (NO), nitrogen dioxide (NO_2), and sulphur dioxide (SO_2) that react with each other in the atmosphere. The effect of such reactions on ground-level concentrations tends to be more important for airshed, ozone, visibility and long-range transportation studies, perhaps over hundreds of kilometres. These are the more common types of applications of atmospheric chemistry. In such cases, the applicability of AUSPLUME and ISCST3 is very limited due to the complexity of the chemistry, and the range over which the receptor grid must the calculated.

In AUSPLUME, the exponential decay of pollutants can be modelled by simply multiplying the computed concentrations by the factor exp(kx/U), where k is the decay coefficient, x is the downwind distance and U is the wind speed at plume height. A single default value for k can be specified for all hours, or a separate value can be specified in the hourly meteorological data file. No other types of atmospheric chemistry can be modelled by AUSPLUME.

A similar decay term is used in ISCST3. The user can specify either a half-life for exponential decay in seconds, or a decay coefficient in units of s-1. A decay half-life of four hours is automatically assigned for SO_2 when modelled in the urban mode.

CALPUFF allows a more detailed simulation of atmospheric chemistry, including transformations between ozone, NO, NO_2 and nitrate (NO_3), and SO_2 to sulphate (SO_4). One of the most common atmospheric chemistry issues regulatory modellers are required to address is estimating NO_2 from modelled NO_x concentrations. This problem is not handled realistically in either ISCST3 or AUSPLUME. Depending on the source, the amount of NO_2 in the exhaust stream as it is released is around 5–10 % of the NO_x. To compensate for the transformation of NO to NO_2 that occurs after the exhaust gases are discharged, modellers have adopted the practice of increasing the amount of NO_2 discharged from the source. In some cases the overly conservative assumption is made that 100 % of NO_x is NO_2.

Expressions by Janssen et al. (1988) have been used quite commonly to estimate conversion of NO_x to NO_2 downwind from emissions, evidently on the mistaken impression that these expressions are based on chemical reaction rate constants. However, the observations and expressions given in the Janssen paper result from the rate of diffusion of ozone into the emission plume rather than the rates of reaction, and in this circumstance Janssen's estimation is probably applicable only to the particular 500 MW power station studied and is of questionable application to other sources.

The method described by Janssen could potentially be useful if local NO_x data are available to estimate how the NO_2/NO_x ratio changes with distance. It may be possible to apply the same observed ratio to the new NO_x emissions to estimate the new additional NO_2.

A conservative method of estimating the extent of conversion of NO_x to NO_2 based on typical background concentrations of ozone and the fast reaction between ozone and nitric oxide has been proposed. The methodology is explained in detail in Appendix C 'Estimation of Nitrogen Dioxide Concentrations from Modelled NO_x Concentrations'. The methodology explained in Appendix C is a pragmatic and potentially very useful way of estimating the rate at which NO is oxidised to NO_2, and is similar to the methodology incorporated into the US EPA ozone limiting model (OLM).

The OLM is conservative for the reasons given in the Appendix, but also because it assumes all the ozone is available to the new source. The OLM will be too conservative when the new source is to be located in close proximity to existing sources. In this case the new source will be competing with the existing sources for the available ozone, and the rate of conversion of NO to NO_2 will not be as great as if the new source was in an isolated location.

It is important to note that either of the methods to assess the production of NO_2 described above may be the more appropriate, depending on the situation being modelled. Further consideration of these methodologies by the wider air quality professional community is required before either may be recommended for general use. This topic will be covered in the *Good Practice Guide for Assessing Discharges to Air* currently under development by the Ministry.

TAPM provides a choice between simple exponential decay in Tracer mode, or more complex chemistry and integrated deposition processes using the Generic Reaction Set (GRS) photochemistry and aqueous chemistry scheme in Chemistry mode. The Chemistry mode uses a similar approach to other urban airshed models, but with fewer species and chemical reactions to allow faster execution of the model. Output species include NO_X, NO_2, O_3, SO_2, PM_{10} and $PM_{2.5}$. The TAPM chemistry scheme is suitable for most applications, and is more comprehensive than some plume/puff models can offer. But for studies that examine the effect of small perturbations to VOC urban emission inventories, a more complex chemistry scheme provided by an urban airshed model is recommended.

Urban airshed models, such as CALGRID and UAM-V, contain a comprehensive treatment of atmospheric chemistry, including reactions between NO, NO_2, O_3 and VOCs leading to the photochemical production of O_3. No assumptions of decay rates or post-processing of chemical output is required. These models are useful on the regional scale, when chemically active pollutants arise from many sources to interact over the urban area (e.g. from vehicles, industrial and domestic sources, and vegetation).

Recommendation 43

When atmospheric chemistry may significantly change the composition of the pollutants contained within the plume being modelled, one of the following methods should be used to assess the changes.

a) Use a Gaussian-plume model if the chemistry can be described by a highly simplified first-order scheme.

b) The model results for inert pollutants may be post-processed to derive concentrations of chemical products. A particular example of this is the calculation of NO_2 from emitted NO_x. (See the US EPA's ozone-limiting method, as described in Appendix C.)

c) Chemistry available in model (e.g. NO_x and SO_x treatment in CALPUFF).

d) A full airshed model should be used for more complex interactions, when many sources are present (e.g. urban traffic, industry, home heating).

The method used to consider the influence of atmospheric chemistry should match the scale and potential effects of the source being assessed. For further advice, refer to the Ministry for the Environment's upcoming *Good Practice Guide for Assessing Discharges to Air*.

5 Meteorology: A Critical Input

5.1 Sensitivity of models to meteorological data

Meteorological data are one of the most important inputs into any air dispersion model. Ground-level concentrations of contaminants are primarily controlled by two meteorological elements: wind direction and speed (for transport), and turbulence and mixing height of the lower boundary layer (for dispersion).

The meteorological data requirements for steady-state Gaussian-plume models and advanced dispersion models vary considerably. Steady-state Gaussian-plume models require meteorology data from a single surface station. They assume that the single station data are applicable to the whole modelling domain up to the top of the boundary layer and that conditions do not vary with height.

Advanced dispersion models – including puff, particle and grid models – allow meteorological conditions to vary across the modelling domain and up through the atmosphere. This is a much more complex situation than for steady-state modelling and thus requires much more complex meteorological data. Because meteorological sites do not provide the relevant data at every point in the modelling domain, a meteorological model is used to predict and provide the meteorological variables at sites where information is not available. The advanced dispersion model then uses this *pre-processed* meteorological data for analysis.

Because the meteorological data requirements vary greatly between these two model types, the choice of which dispersion model to use can depend on questions regarding the expected meteorological conditions. The question, Will the meteorological conditions be uniform across the modelling domain? (or can they be approximated this way?) needs to be answered. You therefore need to consider the:

- boundary layer structure
- atmospheric turbulence
- modelling domain topography
- mesoscale meteorology (air-pollution meteorology).

There is a range of options for collecting and processing land-based meteorological data, including surface meteorological stations, tethered balloons, radiosonde upper air balloons, manual observations, remote sensing systems (SODAR/RASS, Radar, Lidar) and satellites. Various meteorological processors are also available to process raw data into formats required by air dispersion models.

Recommendation 44

Meteorological data must be treated as a critical input for any modelling study.

Steady-state Gaussian-plume models require meteorological data from a single surface station.

Advanced dispersion models allow meteorological conditions to vary across the modelling domain.

5.2 Meteorological data for steady-state Gaussian-plume models

Steady-state Gaussian-plume models require meteorological data from a single site. These data requirements can be met by three approaches, which are discussed in order below. The use of each approach will strongly depend on the:

- meteorological data available
- purpose for which the model is being used
- scale and significance of the potential effects of the discharge
- accuracy of information and level of detail required by the regulatory authority.

The approach taken should match the scale and significance of the discharge being assessed, while making use of the best available meteorological data.

5.2.1 Screening meteorological data

As a first step and when worst-case events are of primary concern, it is generally recommended to use a standard screening meteorological data set as an initial air dispersion modelling assessment. Most commercially available models such as AUSPLUME or ISCST3 supply screening data sets with the model.

Screening meteorological data sets have been developed using standard combinations of wind speed, stability class and mixing heights, which should mimic the range of atmospheric conditions that are likely to occur in any given location. They provide a simple option to run the air dispersion model and can be applied in most locations. The maximum ground level concentration predicted using a screening data set is normally regarded as conservative. This means that it is likely the model over-predicts concentrations expected to occur in reality, assuming that other input data are of good quality. The results from a screening model are often termed 'worst-case scenario' impacts.

There are several limitations to these data. They can only model one-hour averages, not longer time-averaging periods such as eight hours, 24 hours or annual averages. This means that certain contaminants that have ambient guidelines for longer periods – such as PM_{10} (24 hours) – cannot be directly assessed using a screening data set. However, the model CTSCREEN, which comes with a screening meteorological data set, can provide estimates of 24-hour averages.
Another limitation is that these data cannot provide an indication of how frequently an event might occur, what the spatial distribution of the impact is, nor average concentrations.

Screening meteorological data sets should therefore not be used for:

- averaging periods longer than one hour
- PM_{10} sources that are likely to produce significant downwind concentrations
- frequency assessment of pollution events
- airshed sources.

Recommendation 45

Screening data sets should only be used to gain a 'first cut' estimate of the magnitude of the maximum ground-level concentration for a particular source.

When a screening data set is used, the modeller must ensure it contains mixing heights and stability classes which realistically represent the location being modelled.

To estimate the 'worst-case' scenario, all other model inputs, such as emission rates, must be selected and shown to produce 'conservative' results.

5.2.2 Ready-made, site-specific data sets

When screening meteorological data cannot be used, it may be appropriate to use ready-made, site-specific meteorological data sets for modelling. These situations include those when a screening data set does not:

- provide sufficient accuracy
- meet the criteria of the ambient air quality requirements of the local council
- suit the source or type of pollutant being modelled (e.g. PM_{10} from a large coal-fired boiler).

Some urban and regional ready-made meteorological data sets have been produced for some regional councils and are also available for a number of the larger cities in New Zealand (see Appendix B). These regional councils should be able to provide advice on the availability and appropriateness of any ready-made site-specific data set for a specific modelling project.

Some private consultants have also produced site-specific data sets. Normally this data is carefully guarded intellectual property or owned by their clients. But depending on the task for which it is intended and the amount you are prepared to pay, this source of data may be worth exploring. Again the relevant regional council should be able to provide advice on what, if any, data has been produced by consultants for a specific area. The data sets developed by consultants normally cost between $1000 and $5000.

5.2.3 Developing a site-specific data set

If a suitable ready-made meteorological data set is not available or is not applicable to the site in question, one needs to be developed. Provided it is of good quality, on-site data are often the preferred source of meteorological input data even if other nearby sets are available. A distinct advantage of having on-site data is that they can also be used for dispersion model valuation studies.

The predecessor to this Guide is the document *Guidelines for the use of Dispersion Models* (NIWA, 1998). Part 2 of this document provides an overview on the use of meteorological data as input for Gaussian-plume dispersion models. It also contains detailed descriptions of some of the methods used to calculate derived meteorological parameters. While Part 2 of the original modelling guideline provides a useful introduction to the use of meteorological data in modelling, recent developments in meteorological modelling have rendered some of the detail out of date. The following sections provide current recommended practices.

Developing a meteorological data set can be expensive and time-consuming. Depending on the complexity of the site, a degree of meteorological expertise may be required to make sure the data are accurately representing the conditions experienced at the site. It is recommended that if the data are to be used as part of an AEE, they are put through a thorough quality assurance process and/or peer reviewed before use.

The collection of site-specific meteorological data has been fully covered in the documents *On-site Meteorological Program Guidance for Regulatory Modelling Applications* (US EPA, 1987) and Part 51, *Guideline on Air Quality Models* (US EPA, 1999). The former provides details on site location, recording mechanisms, data communication, sampling rates, system accuracies, data handling, quality control and treatment of missing data. It is recommended that this guidance be adopted as best practice for the collection and processing of meteorological data for use in dispersion modelling applications. This is consistent with the approach taken in the *Good Practice Guide for Air Quality Monitoring and Data Management* (Ministry for the Environment, 2000b).

When producing a site-specific data set there are generally two sources of data that can be used: data collected on site, or data collected from an existing nearby source.

a Data collected on site

A meteorological station should be located away from the influences of obstructions such as buildings and trees to ensure that the general state of the environment (wind direction and temperature) is best represented. It is recommended that you use a 10 m high mast for measuring wind direction and speed and temperature differentials. However, where the mast is located in good free-flow conditions and there are height restrictions from local council bylaws, a 6m high mast can be used.

For major industrial sources with tall stacks, or a site within a complex terrain environment, higher monitoring masts (30 m and higher) are recommended to adequately monitor lower boundary-layer wind and temperature profiles. It may be necessary for these situations to supplement or even replace a tall mast with monitoring via remote sensing instruments such as SODAR/RASS or tethered-sonde systems.

On-site data should be reduced to hourly averages for all parameters. To develop a meteorological data set for air dispersion modelling the following parameters need to be monitored from the site:

- temperature
- temperature difference (between 1.5 m and 10 m or higher)
- relative humidity
- wind speed

- wind direction
- solar radiation.

While all the above variables provide valuable information for modelling, the most important variables are wind speed and direction, and temperature. Setting up a station to record and log these three parameters costs approximately $12,000 (in 2004). There will also be relatively small additional costs associated with site maintenance and data management.

Depending on what instrumentation is employed on site, the data collected may need to be supplemented with the following off-site data from the National Institute of Water and Atmospheric (NIWA) Climate Database (CLIDB) system:

- hourly cloud cover and height for the region
- twice-daily upper air temperature, relative humidity, and wind speed and direction from the closest upper air radiosonde station.

When developing a meteorological data set, the representativeness of the data set must be assessed, and demonstrated, in terms of climatic means and extremes. This can essentially be established in two ways: by undertaking long-term (three to five years) monitoring of on-site data collection, or by establishing correlations between on-site data, climatic averages and regional extremes. Average climatic conditions for the region can be obtained from NIWA's CLIimate DataBase (CLIDB) http://www.niwa.cri.nz/services/clidb/.

b Data from locations removed from but close to the site

As a rule, site-specific data are always preferred when developing a meteorological data profile for a specific source. However, sometimes this is not possible or other suitable surface meteorological data from other local sources may be available. For simple single-station plume modelling, off-site data should only be used if the nearby site has similar topographic characteristics which are likely to result in similar meteorological conditions for the site concerned. For example, when both sites are located in the same valley system, or in close proximity along a coastline. The representativeness of off-site data must be established before being used in any dispersion study.

c Where to get raw data from

The three principal sources of meteorological data are:

- Climate Database (CLIDB)
- New Zealand Meteorological Service
- regional councils, which operate ambient air quality monitors.

The Climate Database (CLIDB) (http://www.niwa.cri.nz/services/clidb/) is administered by NIWA in Wellington. Raw data can be downloaded if you are a registered user and familiar with structured query language (SQL). Otherwise NIWA CLIDB staff can download data for an administrative fee. Data are available through a subscription-based web service (CliFlo). Ad hoc or complex data requirements can be requested via the website's 'climate-enquiries' link.

5.2.4 Limitations associated with developing meteorological data sets

Limitations associated with developing meteorological data sets include the treatment of missing data and calm or stagnant conditions. These require careful consideration.

a Calms

Gaussian-plume models assume that concentrations of pollutants are inversely proportional to wind speed, therefore concentrations become unrealistically large as wind speeds approach calm conditions. Two of the commonly used Gaussian-plume models deal with calms in the following manner.

- AUSPLUME calculates pollutant concentrations for a minimum wind speed of 0.5 m/s. Wind speeds in the model's meteorological data input file that are less than 0.5 m/s are substituted with a wind speed of 0.5 m/s.
- ISCST3 calculates pollutant concentrations for a minimum wind speed of 1 m/s. However the criterion of l m/s wind speed is referenced to the point of release (i.e. stack height). Wind speeds generally increase with height above the ground and ISCST3 recognises this. Consequently, depending upon the height of the stack and stability conditions, the wind speeds at point of release may be higher than those recorded in the meteorological data input file (which are generally taken at a reference height of 10 m). ISCST3 does not calculate pollutant concentrations for wind speeds of less than 1 m/s at release height and assigns the concentration for a wind speed of 1 m/s to any hours in the data set where the wind speed is between 0.5 and 1.0 m/s. Any wind speed less than 0.5 m/s is treated as invalid data.

Neither model treats low wind speeds in a realistic manner and effectively throws away worst-case dispersion conditions for many types of sources. If all hours of wind speed less than 0.5 m/s or 1.0 m/s were treated as invalid/missing data and removed from the data set, this may distort the frequency distribution of predicted concentrations. For example, if worst-case conditions are F stability with wind speeds of 0.5 m/s or less and 1% of the data is treated as invalid/missing, then the 99.9 or 99.5 percentile concentration may be very much lower than it would be in reality. For this reason it is recommended that when using steady-state models, all wind speeds less than 0.5 m/s contained in the meteorological data be set to 0.5 m/s. The amount of adjusted wind speed data must be quantified when presenting the modelling results and the potential implications of the data adjustment must be addressed in the assessment.

The potential effect of low wind speeds on assessments undertaken using Gaussian-plume models depends quite strongly on the nature of local wind flow, and the accuracy (or otherwise) of the hourly average wind direction. In some situations, the wind direction may be steady at low wind speeds (e.g. cold drainage flow down-slope or a land breeze), while in other situations the wind direction may be highly variable over a short time scale. In the former situation, the hourly average wind direction may be quite accurate (i.e. the wind direction is quite steady), and the low wind speed prediction from the Gaussian-plume model may be reasonable. In the latter situation, the hourly average assumption results in an over-estimation as the wind direction meanders over a wide range. At any particular site either situation can probably arise at different times. This situation emphasises (again) the value of local meteorological data.

If calm conditions are recognised as a potential issue for a specific site, an advanced model may be used as these still operate no matter how low the wind speed. CALPUFF assumes that

hourly average winds below 0.5 m/s are calms and uses its specific algorithms to deal with them as such. Particle dispersion models, such as that included in TAPM, may give a better picture of dispersion in calm conditions, as they can account for sub-hour fluctuations in the wind and particle distributions are not restricted to being Gaussian in shape. However, there is still some debate on these issues, which remain unresolved.

Recommendation 46

When modelling with steady-state models, all wind speeds less than 0.5 m/s contained in the meteorological data set must be:

a) quantified and reported when presenting modelling results

b) set to 0.5 m/s before modelling.

The implications of not being able to model calm conditions must be addressed in the assessment.

Where maximum concentrations are predicted for low wind speeds, local meteorological monitoring is highly desirable. Use this data to resolve questions about the variability of wind direction and the accuracy (or otherwise) of the hourly average wind direction.

b Missing data

Most meteorological processing programs and air dispersion models require a full data set of all parameters for all hours. Missing data must be replaced with synthesised data to ensure that the air dispersion models can function. Where there are only one or two hours of missing data, linear interpolation of the data is acceptable.

In New Zealand, with many remote automated surface weather stations, longer periods of missing data (in the order of weeks) may occur. For periods of up to seven days, synthesised averages from a longer-term record of the station may be substituted into the data set. For continuous periods of longer than seven days, the data should be considered to be missing and the length of the data set reduced by the length of the missing data. For example, with three weeks of continuous missing data, the total length of the data would cover 49 weeks instead of a standard 52 weeks. It is important, however, to ensure that an adequate coverage of all seasons is obtained within the data.

Recommendation 47

All missing or synthesised meteorological data should be clearly documented and discussed in the method.

Periods of missing data that are less than seven days in length may be replaced with synthesised data produced from long-term seasonally adjusted records.

Periods of missing data that are longer than seven days in length must be recorded as missing data.

5.2.5 Derived meteorological parameters

For steady-state plume modelling there are two key meteorological parameters that are not likely to be directly measured and are required for single-station meteorological files only: stability and mixing height.

a Stability classification schemes

Atmospheric stability is a measure of the propensity for vertical motion and hence is an important indicator of the likely magnitude of pollutant dispersion.

A simplified measure of stability was developed by Pasquill (1961) and later modified by Gifford. This is called the Pasquill-Gifford (PG) Stability Classification and is based on a fairly restricted set of measurements of an unspecified averaging time. The measurements were made in the 1950s. This classification consists of six classes, which include A (extremely unstable), B (moderately unstable), C (slightly unstable), D (neutral), E (slightly stable) and F (moderately stable) (see Appendix A).

In 1967 Turner developed a classification scheme based on the original Pasquill-Gifford scheme. This consists of seven classes including 1 (extremely unstable), 2 (unstable), 3 (slightly unstable), 4 (neutral), 5 (slightly stable), 6 (stable) and 7 (extremely stable).

These classification schemes assume that stability in the layers near the ground are governed by convective fluxes from solar radiation (day), cloud cover (night) and mechanical fluxes from wind speed. Although there are more superior dispersion coefficient schemes, most models offer the P-G dispersion coefficient scheme due to its long and relatively successful history of use.

The Pasquill-Gifford stability classification scheme can be used unless an alternative method can be shown to produce more accurate results.

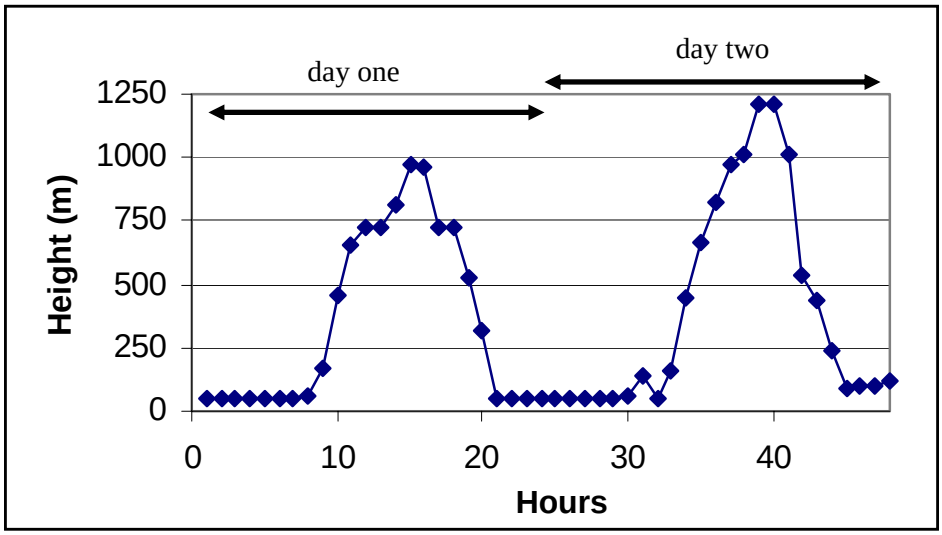
Recommendation 48

Full details of methods used to assign stability classes using routinely monitored meteorological data are given in US EPA, 1987.

b Mixing height

The mixing height or mixing depth is the height to which the atmosphere is uniformly mixed. Mixing height is determined by either upper atmosphere temperature inversions or wind shear (changes in wind speed with height). Mixing heights have a diurnal variation and rapidly change after sunrise and at sunset (Figure 5.1). Research shows an inverse relationship between pollutant concentrations and mixing height, so mixing height is often used as, and is a critical guide of, the pollution potential in an area (Oke, 1987). Dispersion model predictions can be highly sensitive to changes in mixing height.

Figure 5.1: Typical diurnal mixing height variation over two days



If a plume penetrates up through, or is released above, the mixing height, the pollutants will be trapped aloft and their effect will not be observed at ground level. If a plume is trapped within a shallow mixed layer the vertical dispersion will be limited and high ground-level concentrations are likely to occur.

Four methods that are commonly used to determine mixing height are:

- derivation from upper air data (e.g. radiosonde measurements)
- ground-based remote sensing (e.g. Doppler SODAR)
- derivation from routinely measured surface meteorological data (e.g. using a US EPA meteorological pre-processor model such as RAMMET)
- using a prognostic meteorological model (e.g. TAPM, see section 5.3.2).

Determining mixing height is usually an expensive and complex task requiring considerable expertise and should therefore not be undertaken lightly. The uncertainty of mixing heights determined by the methods referred to above increases in the lowest level of the atmosphere. It is generally accepted that mixing heights determined to be less than 50 m contain a significant degree of uncertainty.

Recommendation 49

When mixing height data are required but not available, determine if the model results are sensitive to changes in mixing height by undertaking a sensitivity analysis of the model results to this parameter.

When it can be demonstrated that mixing height data are not a critical parameter, use data that are likely to be representative of the patterns expected in the area of interest.

When mixing height are a critical parameter, derive these data set using the following hierarchy of methods:

a) ground-based remote sensing
b) derivation from upper air data
c) derivation from routinely measured surface meteorological data
d) estimation using a validated meteorological model.

Set the minimum mixing height in a meteorological data set to 50 metres unless there is evidence to show that mixing heights of less than 50 metres do actually occur.

5.2.6 Meteorological conditions that Gaussian-plume models cannot account for

In situations of complex terrain or near coastal boundaries, meteorological conditions such as calms, coastal fumigation, sea/land breeze re-circulation, and mountain and valley winds can significantly affect the dispersion of pollutants. These meteorological conditions are highly complex in a spatial (vary quickly from place to place) and temporal (vary within periods of minutes rather than hours) sense.

Gaussian-plume models cannot account for these meteorological conditions adequately because of the steady-state formulation (which assumes uniform meteorological conditions) and their inability to retain a memory of the preceding hour's emissions. The following examples highlight meteorological conditions that Gaussian-plume models cannot adequately simulate and for which an advanced dispersion model should be used instead.

a Calm and low wind speed conditions

Under stable, high-pressure synoptic (large-scale) weather conditions, calm conditions often occur near the ground, especially at night and early morning. These stable conditions can often result in elevated pollution episodes as vertical and horizontal mixing of the lower boundary layer is inhibited. Calms are of particular concern when dealing with sources that release contaminants close to the ground or when looking at airshed systems. Gaussian-plume models break down during low wind speed or calm conditions due to the inverse wind speed dependence of the steady-state plume equation, and this limits their application. How to deal with calm conditions when using Gaussian-plume models is discussed in section 5.2.5(a).

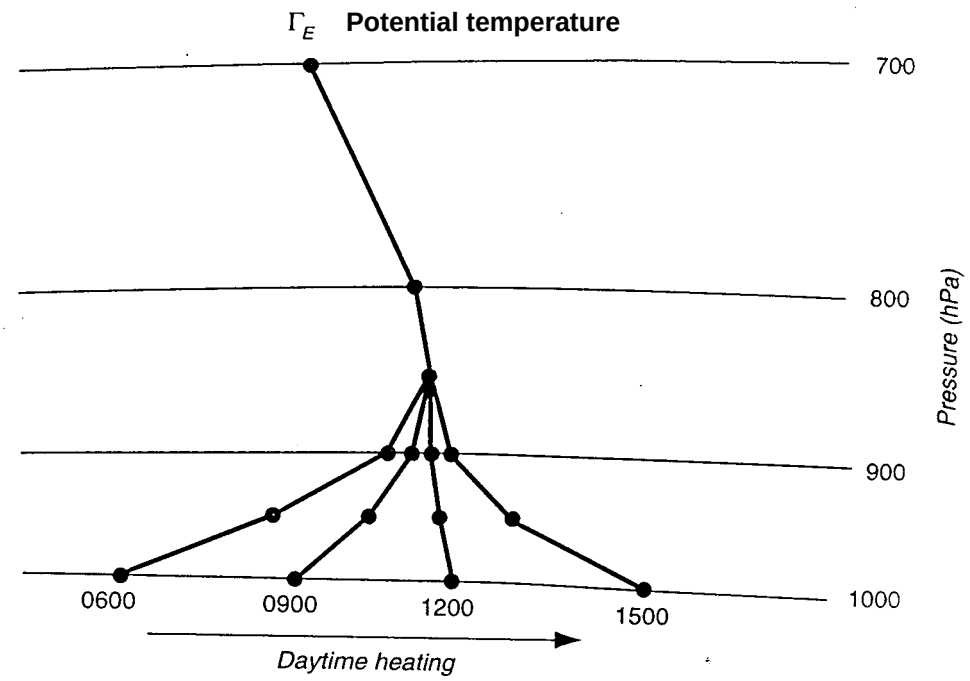
b Inversions

Temperature inversions are caused by a number of different mechanisms. Surface or ground-based inversions often occur on clear, cold nights when there are low wind speeds. Under these conditions the ground cools more quickly than the air immediately above it, causing a pool of cooler, more dense air to accumulate at ground level. These ground-based inversions occur frequently throughout New Zealand, especially in hilly terrain. If temperature inversions develop in a valley, pollutants can often be trapped under the inversion layer and result in high pollution episodes. The break-up of a surface inversion is shown in Figure 5.2, where the layer of air near the ground (at 1000 hPa) heats up during the day by radiative heating while the upper air temperature (above 900 hPa) remains relatively constant.

An advection inversion often occurs when warm air passes over a cooler surface, which can result in the development of a low-level inversion and the formation of ground-level fog. This type of inversion occurs less frequently in New Zealand.

A subsidence inversion or upper air inversion develops within a high-pressure system when the subsiding air is compressed and the upper air becomes warmer than the air below.

Figure 5.2: The break-up of a ground-based inversion during the day



Inversion conditions are difficult to simulate with Gaussian-plume models, due to associated low wind speeds (see section 5.2.7a), the appearance of multiple layers of pollution, and the difficulty of defining the mixing height.

c Fumigation during inversion break-up

Nocturnal ground-based and upper air inversions start to break up during the first few hours of sunlight as the net heat flux (heating of the surface by the sun) becomes positive. As the ground heats from below, convective mixing (heat transfer) takes place, effectively breaking up the ground-based inversion from below. The growing vertical eddies (caused by heating) mix the air above the surface inversion down to ground level, a process called inversion break-up.

Inversion break-up fumigation is the process whereby pollutants emitted above the inversion layer during the night are fumigated down to the ground during this break-up process. Inversion break-up fumigation is often associated with very high pollutant concentrations at some distance from the source. This process is fairly transient, taking place over tens of minutes and typically during mid-morning (Kerman et al., 1982).

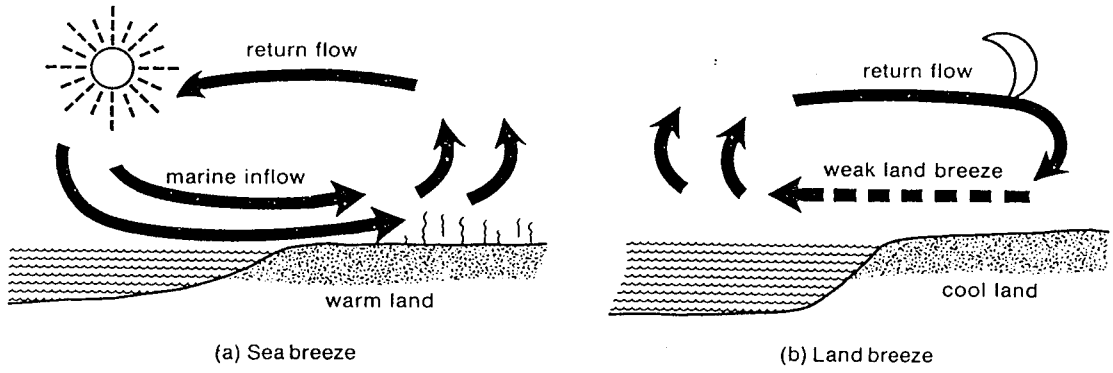
The transient nature of these events, and the difficulties that Gaussian-plume models have identifying different layers aloft and the interaction between layers, makes fumigation during inversion break-up an issue to be wary of when using these models. However, one Gaussian-plume model, SCREEN 3, the US EPA's screening version of ISC3, does incorporate code specifically written to enable it to provide estimates of maximum concentrations during inversion break-up.

d Sea- and land-breeze circulations

Because land surfaces heat and cool quicker than the sea or other water bodies, temperature gradients develop that can result in the generation of localised wind flows (Figure 5.3). A sea breeze develops during the day as the air over the land warms more quickly than the air over the sea. It rises, bringing in an onshore breeze, with a return flow aloft. At night the opposite occurs and a land breeze develops, flowing towards the sea under an area of subsidence.

Sea breezes are generally strongest during the day in summer and land breezes strongest during winter nights. They can both have significant effects on air quality over urban areas, as they are recirculating air currents that can return pollutants (instead of remove them) to an area from which they were released earlier in the day.

Figure 5.3: Sea and land breeze

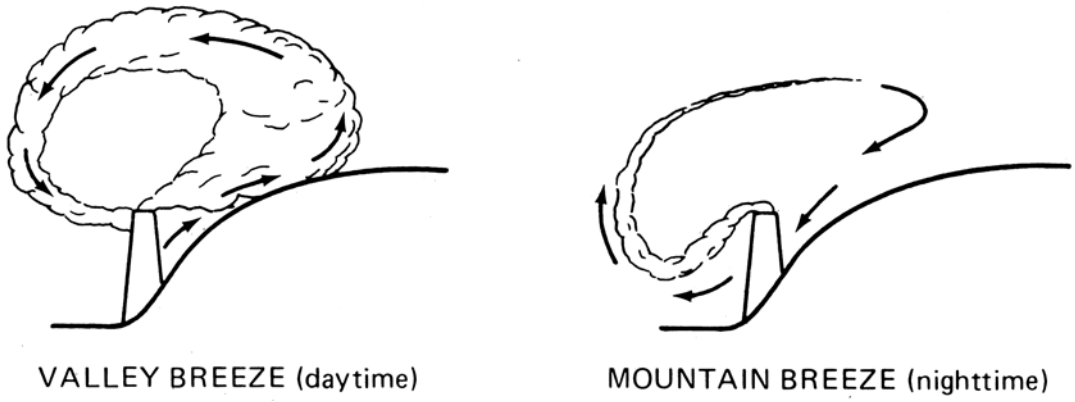


Source: Pendergast, 1984

e Mountain–valley winds

Mountain and valley winds are generated due to similar heating and cooling mechanisms to sea–land breezes. During the day the air above a slope is heated and becomes warmer than neighbouring air at the same height above sea level, but further above the ground. It rises due to convection, and upslope mountain winds occur (Figure 5.4). At night the mountain slopes cool more quickly than the surrounding air, and the cool air drains down the slope, generating valley winds. This heating and cooling often results in closed circulation patterns, which can trap and/or recirculate air pollution in the mountain–valley system.

Figure 5.4: Valley and mountain winds



Source: Pendergast, 1984

Recommendation 50

Where there are meteorological conditions that Gaussian-plume models cannot account for, an advanced model (which is more capable of handling these conditions) should be used.

5.3 Meteorological data for advanced dispersion models

Advanced dispersion models require more complex meteorological data than steady-state models. This includes inputs from surface networks (land and sea) and upper air stations. Because there will not be meteorological sites at every point on the ground in the modelling domain, and monitoring in the upper air (anything above the height of a tower) is normally very sparse, meteorological models must be used to provide this 'missing data'.

There are two different types of meteorological model that can be used to provide a three-dimensional grid of meteorological data:

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

The meteorological model outputs are then used to drive a dispersion model.

Meteorological models can either form part of an air dispersion modelling system (e.g. CALMET provides meteorological fields for CALPUFF, RAMS for HYPACT, and TAPM calculates both the meteorology and dispersion), or they can be stand-alone. Prognostic models (from mesoscale to global scales) are used to provide national weather forecasts. RAMS is used worldwide for this purpose; LAPS – whose analyses are used to drive TAPM – is used in Australia. The NZ Meteorological Service uses MM5 for mesoscale weather forecasts.

Meteorological models of the type described in this section – and their associated dispersion models – have rarely been used in New Zealand for regulatory impact assessments, largely because:

- the models have not been user friendly and needed large computing resources to run them
- the network of meteorological stations for input data to a diagnostic model (especially upper air) is relatively sparse
- the format for data storage is sometimes not compatible with that required by the model.

More recently a number of advanced dispersion models have been released that are much more user friendly. Efforts are always being made by developers to enable models to run faster, and with increased computing power available it is becoming feasible for all users to run these models on a modern personal computer. It is the rapid increase in computing power over recent years that has resulted in an increase in the number of people using these tools.

Examples of diagnostic and prognostic meteorological models are provided in the following two sections. Recommendations outlining which meteorological models to use in the New Zealand situation are given in section 5.3.5.

5.3.1 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. The model’s output is a data file in a format required by a particular air dispersion model.

An example is CALMET, the pre-processor to CALPUFF. In recent years CALMET has been increasingly used in the USA and Australasia, and is used here to illustrate the features of a diagnostic meteorological model.

The CALMET meteorological model (Scire et al., 2000) is a diagnostic meteorological model developed as a component of the CALPUFF modelling system for use in air quality applications. CALMET in its basic form is designed to produce hourly fields of three-dimensional winds and various micro-meteorological variables based on the input of routinely available surface and upper air meteorological observations only. CALMET consists of a diagnostic wind field module and micro-meteorological modules for over-water and over-land boundary layers.

The diagnostic wind field module uses a two-step approach to the computation of the wind fields (Douglas and Kessler, 1998). In the first step, the initial-guess wind field is adjusted for terrain effects to produce a step 1 wind field. The second step consists of an objective analysis procedure to introduce observational data into the step 1 wind field to produce a final wind field, the step 2 wind field. Some of the advantages and disadvantages of this model are detailed below.

Advantages of CALMET

- Observations can be incorporated into the model, to produce realistic meteorological fields.
- CALMET can reproduce fine-scale effects (down to a couple of hundred metres' resolution) and still maintain efficient model run times on a personal computer.
- Output from the prognostic meteorological models such as MM5 and TAPM can be incorporated into the CALMET run, providing information in data-sparse regions. This combined approach is the preferred way of operating CALMET.

Disadvantages of CALMET

- The CALMET/CALPUFF system is technically more advanced than a plume model and is perceived as being difficult to regulate and complex to use.
- Routine meteorological data are sparse in New Zealand.
- There are potentially extra costs of running CALMET.

Summary

With regard to *ease of use*, CALPUFF can be run in a steady-state mode using the same meteorological data that are required to run AUSPLUME or ISCST3. The minimum requirements for CALMET are similar to those for the steady-state models. An ISCST3 or AUSPLUME meteorological file can be used to drive CALPUFF, but again there is the option for a more refined treatment when it is necessary and the data are available.

Costs to industry may be higher for a full CALMET/CALPUFF analysis than a simple steady-state analysis. In many cases, though, the differential is very small compared to other fixed costs of a project, and the differential tends to decrease with increasing modeller experience. Also, a more accurate answer can mean large savings in a project, and in some cases can make the difference between obtaining approval for a project or being rejected. Industry will also save costs from the model's ability to handle multiple effects within one model framework; i.e. once set up the modeller can model anything from long-distance visibility to aqueous phase chemistry to plume visibility applications, without requiring the services and set-up costs of another model.

5.3.2 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 features on scales in the range 1–10 km. Most are run in a nested format with the outer domain covering distances in the order of 500–1000 km – the regional scale.

All domains are initialised using analyses from global or limited-area models, usually run by national weather services. These are provided by many forecasting agencies or similar institutions, such as the US National Meteorological Center, the European Centre for Medium-Range Weather Forecasts, the UK Meteorological Office, or the Australian Bureau of Meteorology. The outer domain is also driven at its boundaries by the global or limited-area models as the run progresses – this feeds in the effects of weather systems to the domain of interest. The prognostic models describe the three-dimensional fields of temperature, wind speed and direction, and moisture through the region at high spatial resolution.

Prognostic models all contain realistic dynamical and physical formulations, and potentially produce the most realistic meteorological simulations for regions where data are sparse or non-existent. The high resolution needed for regulatory assessments means that these models have historically been seldom used as regulatory models. The computing costs of long-term simulations have been prohibitive, although more recently this is less true. And, if local meteorological data are absent, the use of a prognostic modelling system could be a sensible option as part of a regulatory assessment.

RAMS is the most commonly used prognostic meteorological model in New Zealand (Wratt et al., 2001), followed by MM5, ARPS, and (more recently), TAPM.

a RAMS and MM5

RAMS and MM5 are three-dimensional, non-hydrostatic prognostic mesoscale models. MM5 is the fifth-generation NCAR/Penn State Mesoscale model. The model includes a multiple-nesting capability, non-hydrostatic dynamics and four-dimensional data assimilation (Dudhia et al., 1999). MM5 is free to users, while RAMS is subjected to licensing costs. Both models enjoy widespread use throughout the world, are well supported, continually under development, have been used in many studies, and appear regularly in the scientific literature. The main advantages and disadvantages of these models are detailed below.

Advantages of RAMS and MM5

RAMS and MM5:

- have the ability to assimilate local meteorological data
- have realistic dynamical and physical formulations, suitable for simulations in New Zealand's complex environment
- can produce realistic meteorological fields in data-sparse regions
- are flexible enough to couple output meteorological fields to dispersion model runs at any resolution (e.g. RAMS coupled to HYPACT).

Disadvantages of RAMS and MM5

RAMS and MM5:

- have relatively high computational demands
- require a large amount of user knowledge and expertise to produce reliable and convincing results
- do not themselves include dispersion models, and the associated dispersion models do not necessarily comprise all of the features required for regulatory assessments (e.g. building effects).

b TAPM

At present, most prognostic models require significant computer resources to run. They also describe a comprehensive collection of meteorological phenomena and are widely used in meteorological research. However, some features that contribute significantly to the computational cost of mesoscale modelling are not important for air quality simulations, such as gravity waves and complicated microphysical processes. Careful formulation of the model dynamics so as to omit or filter out these features can increase the run speed, enabling longer runs to be contemplated for regulatory applications. This has been done with the CSIRO's TAPM.

TAPM is a PC-based three-dimensional prognostic meteorological modelling system, including various dispersion modules, as described in section 2.2.2. TAPM has a GUI that allows the user to set up and run the model under the Windows operating system. It connects to databases of terrain, vegetation, soil type, sea surface temperature and synoptic-scale meteorological analyses for Australia and New Zealand, as well as most regions throughout the world. TAPM is driven by six-hourly synoptic analyses at approximately 75 km resolution. This database is derived from LAPS analysis data from the Bureau of Meteorology.

Advantages of TAPM

- It is easy to use and completely self-contained, with good visualisation of model results.
- The model output is easy to convert for input into other models, such as CALMET, AUSPLUME, DISPMOD and ISCST3.
- As for any prognostic model, it requires no local data to run, although it has the ability to assimilate local surface meteorological data.
- It is designed to run on a modern personal computer.
- Describes the effects of point, line and volume sources, simulates the effects of buildings on dispersion, and simulates chemical reactions between pollutants.
- Resolution of the pollution dispersion models can be higher than that of the meteorological model – and will usually need to be for regulatory assessments.

Disadvantages of TAPM

- Although easy to use, a high level of understanding of boundary-layer meteorology and pollution dispersion is needed, as with all prognostic model systems, to produce meaningful results.
- The maximum horizontal resolution of the meteorological model component of TAPM is of the order of a 1 km grid-size. If meteorological features are expected, or geographical forcing is present at smaller scales, then the user should take care. Although assimilation of meteorological data is possible, care must be taken to ensure that the meteorological data are representative of the scales modelled by the meteorological model.

5.3.3 Prognostic model output as inputs to Gaussian-plume models

Some prognostic meteorological models produce output data in a format that can be used by plume models. Prognostic model results may be extracted at a single location (the site of pollution emissions) in a format compatible with, say, AUSPLUME or ISCST3, and treated as pseudo-observations for input to the dispersion models. This is a possible alternative if there are no site-specific observations, and has the advantage that there would be no missing data. The pseudo-data would also be compatible with CALPUFF running in a single-site mode. TAPM has options to produce meteorological output compatible with most commonly used Gaussian-plume models.

However, extracting results from a single point to run a plume model ignores many of the advantages of undertaking sophisticated – and more realistic – meteorological modelling, as most information in the prognostic model results would never be used. If a model such as TAPM is being run to produce the meteorological information, then it can be run as a dispersion model at little extra cost.

Care should also be taken when extracting only the mixing height from a single point. Although the model mixing height should be consistent with other model parameters at that location, it may not be consistent with observed parameters (e.g. wind and temperature), which are being used as inputs to the plume model. It would be more realistic to derive the mixing height from meteorological observations.

The practical advantage of extracting single-point meteorological data for a plume model is that the meteorological model need only be run once, no matter how many dispersion model runs are required. As TAPM is a self-contained meteorological and dispersion model, with the two processes running at the same time, the meteorology has to be re-run for each dispersion model case, and this is relatively computer resource intensive. However, other meteorological and dispersion models (e.g. RAMS/HYPACT or CALMET/CALPUFF) carry out the two processes separately. The meteorological data need only be calculated once and this consideration does not apply.

Recommendation 51

Prognostic model output should only be used as meteorological input data for Gaussian-plume models when:

a) it is appropriate to use a Gaussian-plume model for dispersion

b) there is no other source of meteorological data available.

However, using the TAPM meteorological output in a simple (quick to run) dispersion model can be attractive when you want to quickly test a wide range of options.

5.3.4 A combined prognostic/diagnostic approach

Both the prognostic and diagnostic approaches to meteorological modelling have advantages for the production of realistic meteorological fields for input to dispersion models, as follows.

- Prognostic models do not need local meteorological observations to run, so can simulate the meteorology of regions where few data are available.
- Diagnostic models can incorporate available measurements, and – provided the measurements are interpolated realistically – can potentially produce meteorology close to that observed (indeed, at the monitoring sites the modelled meteorology should be exactly the same as that observed).

Two variations on these approaches may be identified in which each model type incorporates the beneficial features of the other.

a Data-assimilating prognostic models

Prognostic models can take advantage of local meteorological data by the process of meteorological data assimilation. There are several ways of accomplishing this. One common method is known as 'nudging'. Essentially, the prognostic model solution is forced towards the observations during the model run. At best, the model solution is already close, so the forcing is small – hence the term 'nudging'. Nudging can have beneficial effects on the model solution, but must be used carefully. For example, the local meteorological data input to the prognostic model should be representative of the observed meteorology on scales resolved by the prognostic model. If the monitoring site is in complex terrain which is not resolved by the prognostic model grid, then its data should not be assimilated.

b Prognostic model output as input to a diagnostic model

Diagnostic models may be run in data-sparse areas through the incorporation of output from a prognostic model. The prognostic model provides a 'first-guess field', which is then modified by the diagnostic model to take account of terrain or land-use features that are at a smaller spatial scale than the terrain used by the prognostic model. The main purpose of this approach is to increase the horizontal resolution of the meteorological fields, which is necessary if there are important terrain or land-use features at the higher resolution. The procedure is far less computationally demanding than running a prognostic meteorological model (with or without data assimilation) at sub-km resolutions.

It is worth noting that:

- approaches (a) and (b) are not new, but they are discussed here as practical approaches to combining results from prognostic meteorological models (which simulate the atmospheric dynamics according to physical laws) with available meteorological observations
- the combined approaches work in both data-sparse and data-abundant regions
- most, if not all, prognostic models have data assimilation routines, so they may be used in approach (a)
- diagnostic models such as CALMET are set up to combine prognostic model output with meteorological measurements in approach (b)
- meteorological observations may be used twice, being both assimilated into the prognostic model run and used in the objective analysis stage of the diagnostic model run.

The choice between approaches (a) and (b) involves considering the best resolution that may be practically attained in a long-term prognostic model simulation. This should be high enough to resolve the important meteorological features which can only be simulated by a prognostic model, such as land and sea breezes, and developing cyclones and fronts. If this is sufficient to resolve terrain and land-use effects on the local meteorology, then approach (a) is appropriate. If there are, say, terrain-forcing effects, such as blocking, channelling or slope flows which are not resolved in the prognostic simulation, then these may be incorporated using a diagnostic model; that is, following approach (b).

It is important to note that the choice between (a) and (b) and the choice of model resolution (for both prognostic and diagnostic) depends on meteorological considerations only. The resolution of the dispersion model is independent of the resolution of the meteorological model(s), and is generally equal to or (much) higher than the resolution of the input meteorology.

These approaches, despite their potential to produce realistic mesoscale meteorological features (which have important consequences for pollution dispersion), have not been widely adopted in New Zealand. They are becoming more common overseas for regulatory impact assessments, and have been used worldwide for many years for scientific research.

Approach (b) involves combining the three-dimensional prognostic model output with meteorological observations (from the surface and from vertical profiles) in a diagnostic model. A variation on this uses a set of key, user-selected vertical profiles, extracted from the prognostic model results, and used as if they were observations in the diagnostic model. The diagnostic model extrapolates to provide three-dimensional fields. The extracted profiles are used in place of the full three-dimensional prognostic model fields. However, three-dimensional model output can occupy an extremely large amount of disk space – files need to be as text rather than binary format so they can be read by a different model. For example, TAPM allows this variation of approach (b) in the extraction of profiles for input to CALMET as pseudo-data.

However, the latest version of TAPM (v 2.0) allows output of the full three-dimensional meteorological fields (as text), which may be converted by the user and read by CALMET.

c Hazards associated with combining model results with observations

Careful checking needs to be carried out with the approach described in section 5.3.4a. Data assimilation works well if the model prediction at the data point is already close to the observation at that location. If this is not the case, the model solution at surrounding and downwind grid points can become nonsensical.

It must be assumed that over a 12-month period the prognostic model will not predict some days well in (probably) all regions. If the intention is to run a dispersion model for 12 months and examine annual statistics, it may be safely assumed that the meteorological model will predict the right types of weather and at the right annual frequency, even if not on the correct day all the time. It is perhaps safer to use the observations to validate the modelled meteorology, rather than assimilating them and potentially generating unrealistic model results. Extra care must be taken if the dispersion modeller wishes to use the meteorological model to simulate a particular day. In that case, the meteorology has to be correct and must be validated against suitable observed data.

Similar considerations apply when adopting the approach in section 5.3.4b. If the prognostic model output used in the initial-guess phase of CALMET's wind field calculation differs from the observations used in the subsequent objective analysis, the resulting wind field will be unrealistic. This can occur particularly if the prognostic model does not resolve terrain effects which are resolved by CALMET. If observations are plentiful, a more realistic wind field may be obtained without the prognostic fields as an 'initial guess'. If scarce, it could be safer to run CALMET in a 'no-observations' mode, where the wind field is a perturbation of the prognostic model output.

5.3.5 The future use of non-steady-state meteorological data in New Zealand

As indicated earlier in the document, an important difference between Gaussian-plume dispersion models and more advanced dispersion models is in their requirements for meteorological data. Advanced dispersion models require fully three-dimensional, time-dependent meteorological data (i.e. 'non-steady state'), which are provided by advanced meteorological models such as TAPM, MM5 and CALMET.

In New Zealand, the creation of non-steady-state meteorological data sets has been mainly carried out by scientists as part of research programmes, rather than consultants with more limited time and resources. This situation is gradually changing, as advanced models are steadily becoming more widely used. This is encouraging, as many dispersion-modelling exercises ought to be carried out using advanced models rather than Gaussian-plume models. Criteria for deciding the kind of model to use have already been discussed.

Once it has been decided that your project requires an advanced dispersion model – and therefore requires three-dimensional meteorological fields – there are several factors to consider when deciding on the most appropriate meteorological model. In other words, there are still some New Zealand-specific issues to address.

For one thing, many areas of New Zealand have very few surface meteorological data sites, and there are only three routine radio-sounding sites providing vertical profiles (Whenuapai, Paraparaumu and Invercargill). This poses a challenge when running a diagnostic wind model using observational data only.

New Zealand's complex terrain poses a different challenge for prognostic meteorological models. As already discussed, attempts at the combined prognostic/diagnostic approach may lead to problems when the prognostic model results are not consistent with observations.

The dispersion modeller, though acknowledging it is necessary, may still be daunted by the task of meteorological modelling. However, in time, as the modelling community in New Zealand becomes more experienced, the consequences of these issues will become better understood, and will be accounted for at the reporting stage. Also, meteorological models are continually improving, and in future they will be able to better handle meteorological conditions in complex terrain and coastal areas.

Finally, it is unlikely there will be an increase in the number of routine meteorological sites around New Zealand.

Recommendation 52

When carrying out non-steady-state meteorological modelling:

a) assess the availability of meteorological data in the region to be modelled
b) consult a topographic map of the region to gauge its geographical complexity
c) determine what spatial resolution is likely to be required
d) decide whether the required resolution is feasible in a prognostic model
e) consider the prognostic model approach if feasible, or else the combined prognostic/ diagnostic approach
f) consider the diagnostic approach alone if meteorological data are abundant
g) take care when assimilating observations into a prognostic model in regions of complex terrain
h) take care when incorporating observations into the diagnostic stage of the combined approach in regions of complex terrain.

These recommendations give only a general indication, and modellers should be guided by their own experience and expertise.

If advanced modelling is necessary, but considered too onerous by the modeller, then the meteorological component should be contracted out, rather than avoided through the use of a Gaussian-plume model.

6 Reporting Modelling Results

6.1 Introduction

The main objective of a modelling study is usually to determine the significance of the effects of pollutants discharged from a particular source. The results must therefore be reported effectively and concisely in a manner suitable for the purpose for which they were produced. This means the results must be communicated in a way that can be understood by other people who may not be experienced in interpreting model output. There are two elements to this: first, to report the modelling results themselves in an easy-to-understand manner; and second, to evaluate the implications of the results in terms of the potential effects of the predicted ground-level concentrations on people's health and the environment (also in an easy-to-understand manner).

This section focuses primarily on the first part – making modelling results easy to understand. The second aspect – how to evaluate modelling results in terms of potential environmental effects and the national environmental standards – will be covered in the upcoming *Good Practice Guide for Assessing Discharges to Air*.

The key factors involved in reporting modelling results are:

- do not include large sections of data in a report, except as an appendix or electronic attachment
- always include information about the input data and how variations may affect the results
- discuss the accuracy of the modelling results
- prepare maps of the pollution contours, where useful
- indicate which factors are most influential in determining the peak ground-level concentrations.

6.1.1 Statistics

Most models allow results to be assimilated and reported in a variety of formats to allow statistical analysis. These include the maximum predicted concentration at each or any receptor, or up to the *n*th highest predictions, where *n* is defined by the user. *n* is chosen to provide commonly used percentile predictions (such as the 99.5 percentile, which is the highest ground-level concentration at each receptor after the highest 0.5% of predictions have been discarded). Tables of the 50 (ISCST3 and CALPUFF) or 100 (AUSPLUME) highest predictions for all receptors can also be generated.

Some models also allow files to be generated that record the number of exceedances of a user-specified threshold value at each receptor. This function allows, for example, the production of graphs or tables showing the percentage of time that model results exceed the evaluation criteria.

AUSPLUME also provides for the generation of a binary file containing all results for all receptors, and in the current version (5.4) of AUSPLUME these data can be processed from within the GUI using the 'statistics utility' to produce percentile data files for the highest, second-highest, and 99.9, to the 90th percentile value.

ISCST3 allows the generation of a 'POSTFILE', which contains all results for all receptors. The postfile can be read by post-processing subroutines such as 'Percent View' by Lakes Environmental (free to download from www.lakes-environmental.com), and used to generate statistical data for each receptor.

Recommendation 53

For the purpose of comparing modelling results to an evaluation criterion:

a) run the model for the minimum period of one full year of meteorological data where possible (i.e. 8760 hours)

b) identify the receptor(s) that are most highly impacted and those that are most sensitive

c) for the receptor(s), report the 99.9 percentile value of the predicted ground-level concentration as the maximum ground-level concentration likely to occur.

Provide an indication of the representativeness of the 99.9 percentile value ground-level concentration by also presenting a number of other percentile values (e.g. maximum, 99.5th and 99th percentile values).

Use the frequency of exceedances to indicate the frequency of 'pollution events' that exceed the evaluation criterion being used.

Reporting the 99.9% predicted value is not simply a case of listing the highest 100 predictions over all receptors and then taking the ninth value on that list. This is a common mistake. The 99.9% value reported must be with reference to a specific receptor, which must be located at the point of highest impact. To ensure that the area of highest impact is identified, it may be helpful to plot contours of both the maximum and 99.9% values. An alternative is to list the ninth-highest value for every receptor and report the highest value identified.

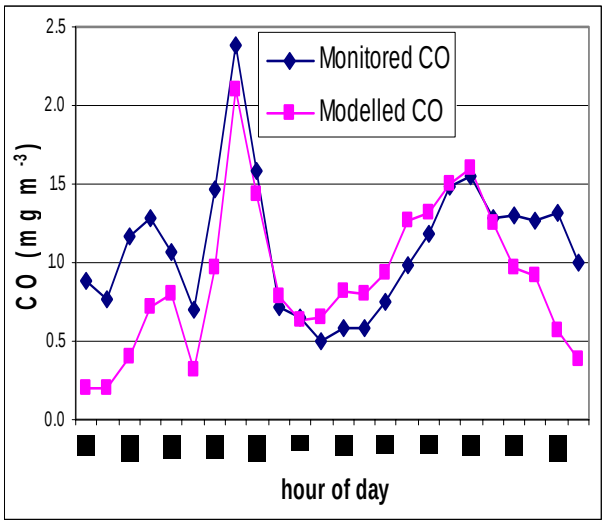
6.1.2 Tabulated results

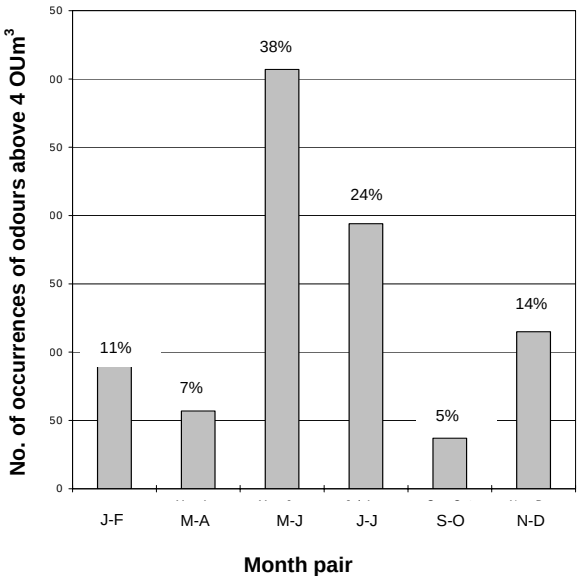
An example of tabulated results from AUSPLUME for the highest ground-level concentration at each receptor is shown in Table 6.1. ISCST3 and CALPUFF files show a similar format. This table shows that the highest ground-level concentration (in these grid locations) is located 10 m East, 70 m North, was 0.809 (concentration units) and occurred at 8 pm on 18 May 1997. Such data can be imported into spreadsheets like Excel or Lotus and sorted to analyse for seasonal or daily trends (Figure 6.1).

Table 6.1: Example of tabulated results in AUSPLUME

Highest recordings for each receptor (in concentration units)				
Averaging time = 1 hour				
X (km):	0.000		0.010	
Y (km)				
0.100	2.79E-01	24,27/02/97	2.93E-01	24,27/02/97
0.090	3.57E-01	24,27/02/97	3.71E-01	24,27/02/97
0.080	4.64E-01	20,18/05/97	4.79E-01	24,27/02/97
0.070	7.64E-01	20,18/05/97	8.09E-01	20,18/05/97

Figure 6.1: Examples of analysis for daily and seasonal trends





6.1.3 Graphical results

Models can generate data files for importing into a graphics programme. ISCST3, AUSPLUME, and CALPUFF (via the post-processing programme CALPOST) all produce data files summarising the results in an 'x, y, z' three-column ASCII format (x co-ordinate, y co-ordinate, concentration) suitable for importing into SURFER for graphical analysis. SURFER is the most commonly used plotting programme with dispersion models. AUSPLUME links directly to SURFER for graphical utilities within the AUSPLUME GUI.

Spreadsheets such as EXCEL are also used for graphing one-dimensional data from screening analyses, such as that shown in Table 6.1.

Following are some suggestions for preparing graphs in SURFER from modelling simulations.

Set the number of points in the SURFER grid to be the same as your number of receptors (section 4.2.2).

Overlay the graphed concentration contours with a base map and terrain map (if appropriate) to allow people viewing the graphs to understand perspective, scale, and context of the results (e.g. 'Where's my house in relation to this?'). If you do this, make sure that your scale is the same on both the contour map and the base map, and if possible overlay the two maps onto the same axes using the 'Overlay Maps' function.

Remember that SURFER is simply a mathematical interpolation programme that draws contours of best fit between your data points. If your number of data points is low, the interpolation may look poor. Pockets of concentric circles often indicate an anomalous data point which is out of place compared to neighbouring receptors, and the data file used to create the graph should be checked.

If you have multiple source groups in your model, then AUSPLUME lists the results for each group one after the other in the same plot data file. These must be divided into individual plot files using a text processor before importing into SURFER.

SURFER will allow you to calculate the area of a receptor grid that is impacted by concentrations above a user-defined level. This can be a useful tool if you want to explore the extent of impact as well as the magnitude.

'Percent View' by Lakes Environmental (free to download from www.lakes-environmental.com) can be used to generate percentile plots (up to 99.0%) for whole ISCST3 grids, (Figure 6-2 and Figure 6-3).

Results of the top 100 (say) predictions can also be used to generate detailed percentile statistics at any given receptor by making the grid so small that it only includes one receptor at the location you're interested in. The results table then shows the top 100 results for that receptor, which can be used to calculate the 99.9, 99.0, 98.0, 95.0 percentiles, etc, and graphed (Figure 6-4).

Similar statistical post-processing options to those in ISCST3 and AUSPLUME are available in CALPUFF's post-processing program CALPOST.

Figure 6.2: Example of a contour map overlaid with a base map

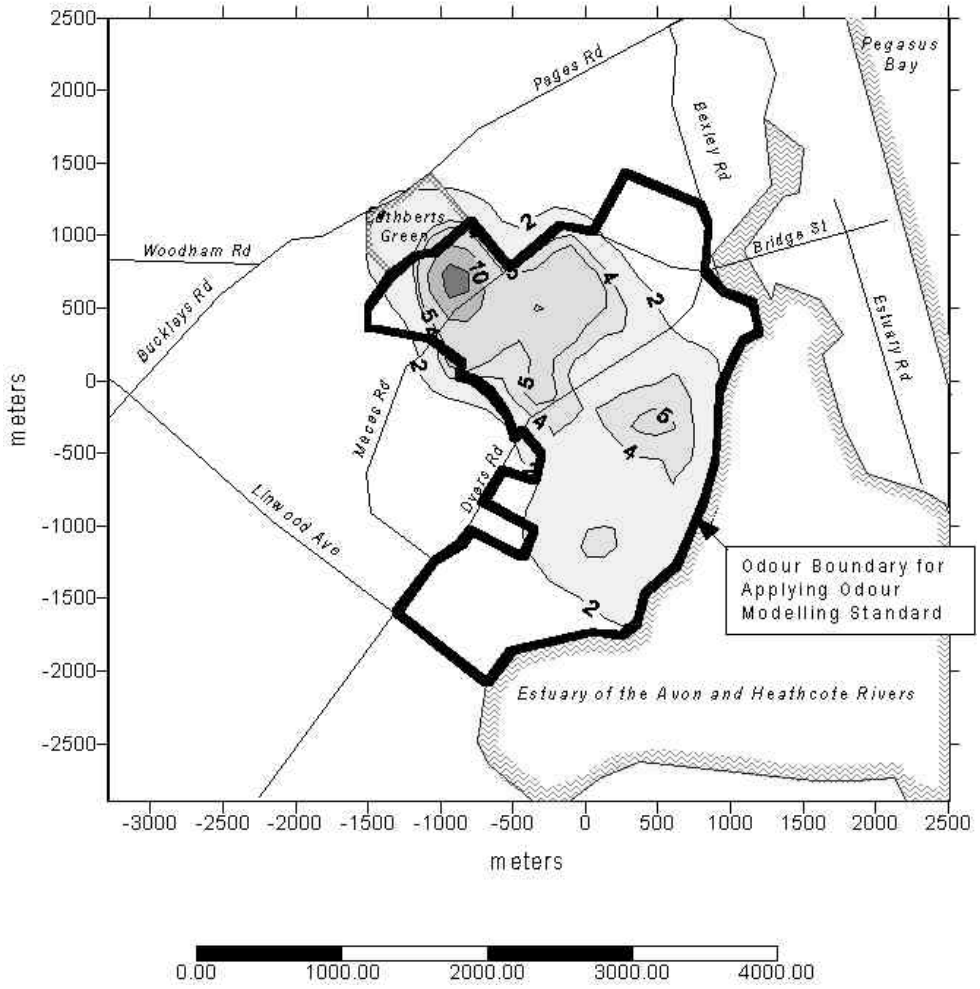
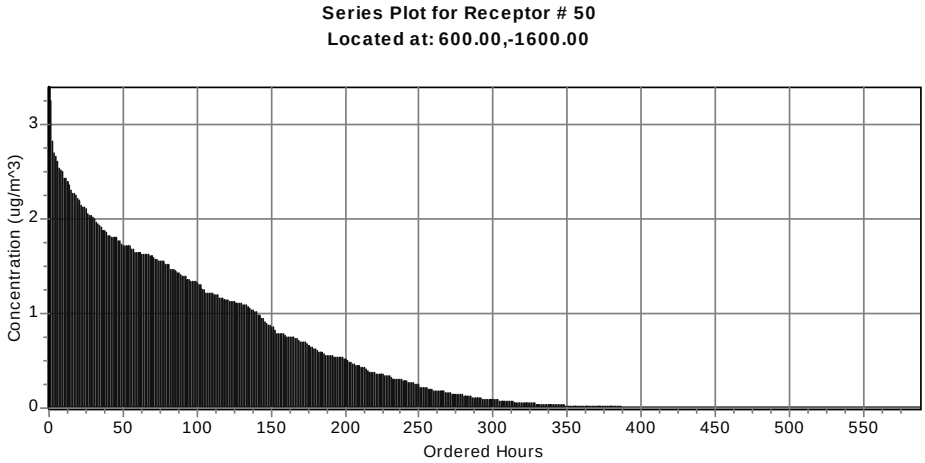
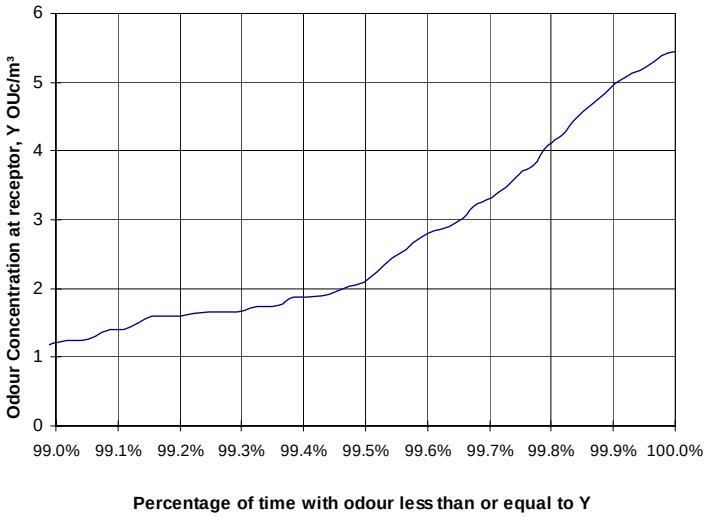


Figure 6.3: Series plot for a single receptor generated by Percent View



Source: Lakes Environmental.

Figure 6.4: Example of percentage occurrence analysis at a single receptor



Recommendation 54

Present modelling results graphically whenever it is helpful and appropriate.

Use sufficient labelling and include legends to allow people without expert training or experience in dispersion modelling to understand the data.

If presenting contour plots:

a) indicate the location of sources, site property boundary and potentially sensitive receptors

b) keep the number of concentration contours to the minimum necessary for conveying the information

c) include the relevant evaluation criteria

d) paste the contours over a map or photograph of the impacted area

e) calculate the area of a receptor grid that is impacted by concentrations above the evaluation criteria. This is a useful tool if you want to explore the extent of impact as well as the magnitude.

Present a percentage occurrence analysis for sensitive receptors.

Present graphs showing the daily and seasonal variation of the ground-level concentrations caused by the contaminants discharged from the source.

Include the plot file data as an electronic appendix to the report.

6.2 Accounting for and reporting of model error and uncertainty

One of the most common criticisms of dispersion modelling is, "It's not at all accurate – it's only a model". To avoid such criticisms it is important to follow some simple principals, as listed in the recommendation box below.

Recommendation 55

Design all modelling studies to be as accurate as possible for the purpose of the study.

Allow the accuracy of the modelling study to be easily assessed by:

a) stating the objectives of the study
b) demonstrating that the model inputs are as correct as possible
c) knowing and stating the model performance limitations
d) demonstrating (via the methodology) that the modelling process has been conducted appropriately
e) including any validating information from monitoring that might be available.

If corners are cut on any of these, the results can be at best meaningless, and at worst dangerous, especially if they are used to justify an important decision. There are three main general sources of error and uncertainty in dispersion modelling:

- inaccurate input data
- inappropriate use of the model (or expecting too much from it)
- poor performance of the model itself.

The total uncertainty contained in the model results is the cumulative effect of these sources. It is useful here to distinguish between 'reducible' and inherent uncertainty. Reducible uncertainty includes the accuracy of the input data (sections 6.2.1 and 6.2.4), and the way in which the model is run (sections 4 and 6.2.3). The inherent uncertainty is the fundamental limitations in the way a model works. This is beyond the control of the model user but is an issue they must be aware of (section 6.2.2).

6.2.1 Input data uncertainty

Any model is only as good as the input data. But of course the question is always: how good does it need to be?

There are three sets of data needed for dispersion modelling:

(a) source, or emissions characteristics,

(b) meteorological data, and

(c) terrain and local features data.

a Source characteristics

The critical factor is to know the rate of emissions, in mass units (grams per second or kilograms per hour or tonnes per day), of the contaminant of interest. This needs to be known for each time period of the model run, usually hourly for a year. Only in very special cases is this constant and known accurately. There are several possible approaches.

- The most common method, which is usually easy to achieve and justify, is to use the maximum emission rate. This occurs when an appliance is operating at its upper limit (e.g. a coal boiler consuming the maximum amount of fuel for which it is designed). If the emissions are measured by an 'approved' method, this is ideal. Guidance on emissions monitoring methods can be found in the Ministry's *Compliance Monitoring and Emissions Testing of Discharges to Air* (MfE, 1998). If actual emissions measurements are not available, then either a manufacturer's design specification or an emission factor (refer section 4.1.2) can be used.
- Another method, applicable in many circumstances, is to use a percentile discharge rate – either 99.9%, 99.5% or even 95%. This is common in processes that can have occasional upset conditions, such as a wastewater plant malfunctioning. Using the upset rate can bias model results severely, leading to predicted concentrations that might be far higher than are ever likely to occur because the particular combination of discharge and meteorology leading to these concentrations might be very rare. This should be investigated and the use of a percentile discharge rate should be clearly justified.
- A method occasionally used is to measure rates that vary by time of day, day of week, or season. Some processes do not discharge all the time, and modelling that takes account of this is more realistic.
- For processes where there is a known hourly discharge rate, in theory these can be directly input into the model, along with the concurrent meteorological information, to produce a very accurate assessment. In practice this is almost never done. This level of accuracy in emissions rates is usually not warranted, as the uncertainties in other factors (meteorology, terrain, model performance) take over.

The overriding feature is that peak modelled ground-level concentrations will be directly related to the emission rate, so it is important:

- to use a rate that is sufficiently large to cover the worst-case discharge of concern
- that the period the maximum emission lasts for matches the averaging period of the relevant evaluation criteria.

Recommendation 56

Clearly state the value and the origin of the source characteristics data that have been put into the model.

Include a copy of the model input file as an (electronic) appendix to the report.

Justify your choice of a particular value of a parameter, or run the model with a range of possible input values.

Preferentially use measured source characteristic values over estimated rates or emission factors.

If using calculated source characteristic values, clearly state the method used to calculate the value. Provide detailed calculations in an appendix to the main report and explain potential uncertainty with the values.

Pay particular attention to emission rate data by:

a) using a rate that is sufficiently large to cover the worst-case discharge of concern

b) ensuring the period the emission lasts for matches the averaging period of the relevant assessment criteria.

Provide a sensitivity analysis of model results to variation in source characteristics. This can be done by running the model with the two extreme values of a particular characteristic (e.g. low and high efflux velocities).

Facilitate an independent review of the source data and avoid requests for further information by reporting all sources of data and assumptions made.

b Meteorological data

Lack of appropriate meteorological information is often the single most important limiting factor in modelling accuracy. It is also the most subjective in deciding just how many data are needed, from which location and how accurate they must be.

The ideal is to have at least one year of data, with at least hourly resolution, at the site of interest (usually within a few hundred metres). The minimum measurement requirements are for wind speed and direction, but some method of estimating stability and mixing height is also required as an input for steady-state modelling. A full description of the meteorological detail is contained in section 5.

Often there are no suitable meteorological data at all. In this case, a 'screening' modelling study using a theoretical meteorological data set can be done. This will uncover the worst-case situation, and show the highest concentration that might occur. However, it gives no information on the frequency or location of the peak concentration, nor on the percentile statistics. When the predicted maximum ground-level concentration is well within the evaluation criteria, the use of a screening model may be sufficient. However, where the predicted ground-level concentration is higher than the evaluation criteria, a more thorough modelling study may be required and more accurate input data (including meteorological and emissions data) will be needed.

For each step in improving the meteorological data, the accuracy and reliability (and 'modelling believability') of modelling results improves. Possible improvements include:

- a simple mast with basic monitoring equipment in the general vicinity
- a simple mast at the site
- a well instrumented mast
- an array of masts
- full vertical sounding data
- model-generated data (using mast and/or sounding data)
- periods longer than one year
- previously used data sets (with accuracy confirmed in previous studies).

When the site is not uniform, further problems can occur. This frequently happens in New Zealand. For instance, the plume is influenced by meteorological conditions that are not the same as those at the site. Winds at plume height may be different from those at the surface, sometimes substantially so. There are also more subtle problems with conditions changing during the modelling period. Some models can handle this (especially puff models), but additional detail in the input data is required.

The required accuracy of modelling results and input data is guided by national guidance in this document and the *Guide to Assessing Discharges to Air* (currently under development), requirements in regional plans, recommendations from council staff and reviewers, and legal/council precedents. A key component of this system is often the use of independent reviewers of modelling, particularly in cases where there is an indication that some contaminant concentration is close to, or exceeding, the evaluation criteria. To assist councils, reviewers and modellers, some key principals should be followed when deciding on and reporting information about the level of detail in the meteorological input data. These are given in the recommendation box below.

Recommendation 57

Clearly state the origin of the meteorological data that have been put into the model.

Minimise the meteorological input data uncertainty by following (as far as practicable) the recommendations made in this document in section 5.

Facilitate an independent review of the meteorological data by reporting all sources of data, assumptions made and any guideline recommendations not followed.

Assess the sensitivity of the model's prediction of the magnitude of the maximum ground-level concentration to meteorological input data. Do this by running the model with data from a number of years, or data from a site with similar climate and meteorology. A comparison with results obtained using screening data can also be useful.

Include a copy of the meteorological data file(s) used as an (electronic) appendix to the report.

c Terrain and other local features

As discussed in section 4.3.4, dispersion modelling requires information about the terrain features surrounding the site that affect dispersion and plume behaviour. These include:

- terrain descriptions
- the location and size of hills
- building features
- surface features such as roughness length
- heat flux (for some models).

Determining the required accuracy for terrain and other local features is quite subjective. In many cases the decision is determined by what is available rather than what is required. It is also very dependent on the application; for instance, for mildly buoyant sources with low stacks, the building downwash issue can be critical, and building dimensions and orientations will determine the accuracy of the model prediction. At the other extreme, for hot, buoyant sources, discharged through tall stacks with final plume heights above 100 m, the building dimensions are irrelevant.

Similar arguments exist for each of the other parameters, and so the effect of terrain information on the accuracy of the model will vary between different applications.

Recommendation 58

Clearly state the origin of the terrain data that have been put into the model.

Justify your choice of a particular value of a parameter, or run the model with a range of possible input values.

Quantify the influence of terrain information on the model results in any particular application by performing an analysis of the sensitivity of the model results to each terrain parameter (section 6.2.4c).

6.2.2 Model performance

After input data uncertainty, the fundamental limitation for dispersion model accuracy is the way the model works. This includes the structure, physics and chemistry, and the way these are all parameterised and computed. There is considerable debate over this, as can be attested by anyone who has attended a technical meeting of model authors, and watched them defend their model's features!

In theory, it should be possible to evaluate any model's performance by a formalised evaluation scheme, whereby it is compared with actual monitoring results (with all other things being equal – emissions rates, meteorology and terrain). Indeed this is done to compare different models. However, in practice this is a complex and expensive process, and virtually impossible for all circumstances. The issues associated with evaluating model performance are outlined in detail by Hanna (1988) and Weil et al. (1992). More recently, model validation has been addressed by the initiative on the Harmonisation within Atmospheric Dispersion for Regulatory Purposes (http://www.harmo.org/). One of the outcomes of this initiative has been to produce the

so-called *'Model Validation Kit'*.[1] This kit is a collection of three experimental data sets accompanied by software for model evaluation.

Most of the commonly used models have undergone some form of validation of their performance. It is recommended that model users should familiarise themselves with the relevant literature before using and presenting results from a particular model. Table 6.2 contains examples of the validation studies that have been undertaken.

Table 6.2: Model validation studies

Model	Authors (year)
ISCST3	Hall et al (2002)
ISCST3	Riswadkar and Kumar (1994)
TAPM	Luhar and Hurley (2003)
TAPM	Luhar and Hurley (2002)
CALPUFF	Strimaitis and Chang (1998)
CALPUFF	Tolga (2003)

One of the most commonly applied models in New Zealand, AUSPLUME, does not have an extensive series of formalised evaluations, instead relying on its similarity to standard Gaussian-plume models, such as ISCST3, which have been validated. One of the validation studies of AUSPLUME that has been completed (Bluett, 1998) shows that the model's performance in New Zealand is generally within a factor of two and similar to that observed in overseas studies.

A further complication exists in New Zealand, where many cases have complex terrain features. Complex terrain is handled poorly by Gaussian-plume models, and where it is an issue advanced models should be used. In theory, advanced models should give very accurate results provided adequate input data are available.

It is typically accepted that accompanied by good input data, dispersion modelling may be used to predict concentrations within a factor of two.

[1] http://www.dmu.dk/atmosphericenvironment/Harmoni/M_V_KIT.htm.

Recommendation 59

The 'factor of two' performance guideline is probably still applicable to Gaussian-plume models. In the interim or until the model is validated, it is probably a safe estimate of likely model accuracy.

If the model shows that the peak concentration is less than half the evaluation criteria, then it can be accepted with a good degree of confidence that the criteria will not be exceeded.

A result showing, say, just 20% under the evaluation criteria is not enough evidence to show that the relevant criteria will not be exceeded. Further evidence, such as conservative inputs or validation of model results against monitoring data, should be used to demonstrate the robustness of results that are relatively close to the guideline (or national environmental standard) value.

Greater confidence can be placed in the results of well-validated and well-executed plume and puff models that have accurate input data.

Until greater general experience is gained or some further formal validation studies are completed, it is not possible to say how much more confidence can be given to well-executed plume and puff models.

Model performance should be regarded as better in simple compared to complex situations (e.g. flat compared to hilly terrain).

6.2.3 Misapplication of models

A common, but largely avoidable, source of modelling uncertainty is a model being used inappropriately. Some cases of this are:

- using a Gaussian-plume model to predict effects on a steep hill
- ignoring building downwash for a short stack on a large building
- using the output from screening modelling to produce a percentage exceedance (yes it has been done!)
- using a default meteorological data set that comes with the model (and is from the other side of the world to New Zealand)
- having the wrong default values in the user settings (such as a 0.1 m roughness length over an urban area when it should be 1 m or even 2 m)
- editing input data sets (particularly meteorological files) to remove conditions that lead to high concentrations
- assigning too much accuracy to the model output (e.g. "The modelled peak is 348, which is less than the 350 guideline, so its fine").

There are no specific recommendations to avoid these problems, except to approach all modelling results with caution and to seek further information where anything is not clear. However, provided modellers have reasonable experience and clearly document the model development and analysis of results, any misapplication of models should be avoided or picked up by the council assessor. Misapplication can also be avoided by discussing modelling options with the council assessment officer before commencing the modelling exercise and submitting the assessment of environmental effects.

Recommendation 60

Avoid misapplication of models by clearly documenting the development of the model and the analysis of its results.

6.2.4 Minimising errors

Despite the limitations discussed above, there are several practical steps that can be taken to minimise uncertainty in modelling results.

a Check, check and check

It is remarkably easy to get one or more inputs wrong. Figures get transposed, formatting is not right, there is poor quality control on input files, revised output gets overlaid on old outputs, plotting results on maps are in the wrong place – even things like using northern hemisphere co-ordinates because they are the default. Many of these errors can propagate into the final results. There is no substitute for checking. As a general guide, it is worthwhile spending almost as much time checking all the inputs and data used as setting up and running the model. Methods that can be used to check input files and output data are provided in section 6.3.

b Sensitivity analysis

Another more formalised way to assess model result uncertainty is to conduct a few extra runs with slightly changed parameters. What if we make the stack slightly higher? What if we restrict minimum mixing heights to 50 m instead of 30 m? What if we 'move' the source 100 m further out? What if we change the roughness length from 0.5 m to 1 m? Each of these actions should have a broadly predictable effect on the results If this isn't as expected, something may be wrong. This analysis determines which are the important parameters; that is, those to which the model results are most sensitive. These are the parameters that need to be known with the most certainty.

c Percentiles

Model results are increasingly presented in terms of percentile exceedances, rather than absolute maximum results. This makes the results more robust, and probably more realistic for what people want out of the modelling assessment. Ground-level concentrations at any particular receptor may be highly skewed. The absolute worst hour may have a concentration twice that of the second-worst hour, and 10 times that of the ninth-highest. However, the ninth-highest may only be fractionally above the tenth-highest. This means the modelling result which is taken out and used (often just a single figure) is greatly sensitive to modelling uncertainty when it is the peak, but much less so when it is the 99.9 percentile.

Recommendation 61

Use an independent person review (and perhaps cross-check) all of the model inputs and outputs. It is not sufficient for the reviewer to consider the final hard copy of the report.

Check model results for 'realism' (e.g. diurnal or seasonal variation).

Where appropriate, perform a sensitivity analysis by conducting extra model runs with parameters changed to reflect the extremes of any particular parameter (e.g. high and low efflux velocities).

Present results for the maximum concentration and a range of percentile statistics to provide an indication of the sensitivity of the maximum ground-level concentration to the model inputs.

6.3 Analysis and interpretation of model results

Once the modelling has been carried out, the results should be analysed to ensure they are believable – at this stage there may still be errors in the model configuration that have not been found (or could not have been predicted). Although the user is often guided by experience, there are a several checks that should always be carried out.

Are the highest concentrations in the right location?

- Expect peak concentrations very near the source for low-level emissions.
- Expect peaks further downwind of tall stacks.
- Expect peaks on terrain features as plumes impinge on them (although these may not be realistic in a Gaussian-plume model if the hill is too distant).

Are the highest concentrations consistent with the meteorological conditions?

- Expect peak concentrations from tall stacks during convective/fumigation conditions.
- Expect peaks from low-level emissions during stable conditions (e.g. night time).
- Check how the concentrations vary with wind speed, taking care with calm periods.
- Check whether the highest-ranked concentrations occur at the same time, but at different locations (receptors), and are therefore occurring under the same meteorological conditions.
- Group the highest-ranked concentrations according to location, time of day and meteorological conditions to determine whether they are clustered into pollution 'events'.

Do the highest concentrations coincide with the maximum emissions?

- If the emissions are time-dependent, look at the relationship between times of maximum emissions and times of highest concentrations.

Are the highest (and lowest) concentrations consistent with air quality observations?

- If air quality observations are available, and the model results provide a good match at the monitoring site, then confidence in the model to simulate pollution levels elsewhere is increased.

When using non-steady-state meteorology: are the important conditions simulated well by the meteorological model?

- Quantify the extent to which the dispersion model results are affected by meteorological model performance.
- If high concentrations are expected during, say, sea-breeze conditions, slow valley-drainage flows or pooling of still air, check that the meteorological model gives a realistic representation of such conditions.
- Check whether peak concentrations occur during these conditions, both in the model and in the observations (if any).
- If the model performs poorly in these conditions, take steps to improve the meteorological simulation (through changes in the meteorological model configuration).

These considerations will help the interpretation and provide information that can be used to validate the model results. They will also help to determine the relationships between pollution levels, meteorology and emissions. Finally, if required, the above considerations will enable predictions of what would happen under alternative scenarios. Any predictions should be tested through further model runs, which might incorporate changes in or redesign of the emitters; for instance:

- restriction of operation times
- changes in stack height, stack location or fuel type.

Most emission options will probably have been specified in advance, but the modelling may be used to indicate other options. These tests are in addition to the sensitivity studies described above.

Recommendation 62

To provide a full interpretation of the results provided by any dispersion model:

a) carry out an analysis of the dispersion model results, ensuring that periods of extreme concentrations are consistent with the meteorological conditions, geographical situations, source configuration and emission rates
b) examine the relationships between concentrations, meteorology and emissions
c) compare the dispersion and meteorological model results with observations (if available).

6.4 Accounting for background concentrations

While there is usually a case for assessing the effects of a particular discharge, people are more interested in the overall end result – the cumulative effect. The Resource Management Act 1991 also requires this, and it is spelt out in most regional plans.

This means that modelling results must be added to current background concentrations discharged by other sources. It sounds simple, but there are many issues to deal with, including:

- If background data concentrations are available, how should they be used?

- What if there are no background data?
- Do maximum predicted and monitored concentrations occur at the same time of the day and under the same meteorological conditions?
- Should the concentrations just be added?
- Should we use peak values or average values, or something else?

More detailed guidance on dealing with background concentrations will be provided in the upcoming *Good Practice Guide for Assessing Discharges to Air*.

Recommendation 63

Modelling assessments must take into account the potential cumulative effects caused by the addition of the discharge being modelled to the current background concentrations.

6.4.1 When local air quality data are available

Having suitable data on background concentrations is an ideal, but uncommon, circumstance. However, the general rule is that anything is better than nothing, and it is worth obtaining whatever data are available from a monitoring site as close as possible to the discharge. Typical sources of data include:

- the National Air Quality Database (http://aqdb.niwa.cri.nz/)
- the Ministry for the Environment's Global Environmental Monitoring programme (Auckland & Christchurch only)
- the Ministry for the Environment's Air Indicators web pages (http://www.environment.govt.nz/indicators/air/)
- regional, district or city council state-of-the-environment reports
- regional, district or city council monitoring programmes
- reports on specific monitoring programmes
- research data (universities and Crown Research Institutes)
- published papers
- consultants' reports (on consent applications)
- industry monitoring programmes
- airshed modelling.

The type, quality and representativeness of these data sets vary enormously, and it is very important to understand what has been measured. In conjunction with the air quality monitoring data, it is also important to get hold of any meteorological monitoring from the site as well. This information can help to determine whether the peak background concentrations occur under the same conditions as the peak modelled predictions.

Recommendation 64

When available, use locally recorded air quality data to assess background levels.

The use of background data for cumulative effects assessments should be accompanied by a discussion of its applicability for the intended purpose.

If there is any doubt as to the validity of the information, it should not be used without specific justification.

Meteorological data from the monitoring site should also be examined when assessing the background monitoring results.

6.4.2 When local air quality data are not available

In most cases, an assessment of cumulative effects is required, so background concentrations need to be estimated. Options for estimating background concentrations are discussed below.

a Model other sources

In some cases it is viable to explicitly model the likely cumulative ground-level concentrations caused by other sources in the area. For instance, if the issue is how a particular plant's emissions affect an area that only has one or two other sources (even if these are complex, such as a roadway), then the modelling can include these sources.

b Compare the location with somewhere similar

If the area does not have significant large sources, and does not have any complex geographical or meteorological features, then it can be assumed that the air quality will be similar to another area of similar population density, emission sources and meteorology. This method requires that such an area can be identified, and that monitoring data are available.

c Make a worst-case assumption

In the absence of any of the above it might be necessary to simply 'guess' the existing air quality. The safest guess is to assume a concentration that is at the upper end of what might be feasible, based on what is monitored in, say, Auckland or Christchurch. As an example, it is almost inconceivable that summer background PM_{10} concentrations in a small town would be greater than those found in the middle of Auckland, so it is reasonably safe to use the monitored values from Auckland. However, the fact that this approach is potentially overly conservative should be taken into account in the assessment.

d Start a new monitoring programme

If all else fails, or if the issue is likely to be of significant importance, start a new monitoring programme as soon as possible. This need not be expensive, as useful information can be

gained from relatively short-term surveys, or from passive monitoring. Comprehensive guidance on setting up ambient air quality monitoring stations is provided by the Ministry for the Environment in the *Guide to Air Quality Monitoring and Data Management* (Ministry for the Environment, 2000b).

Recommendation 65

When locally recorded air quality data are not available, one or more of the following methods should be used to estimate background concentrations:

a) Model other sources to provide an estimate of background concentrations
b) Use data from a similar location affected by similar discharges and meteorology
c) Make a worst-case assumption of background concentrations
d) Start a new monitoring programme to accurately determine background concentrations.

6.4.3 How to incorporate background data

Once background air quality data and model results are available, adding the two together to provide an estimate of the cumulative impact of the discharge provides the most conservative result. However, there are a number of issues with this approach, and in some circumstances a different method is preferable.

a Spatial co-incidence problems

It is often difficult to know whether the background data are representative of the point at which the modelled peak occurs. In general they will not be, leading to an overestimate of the cumulative effect. However, provided the overestimate is within the evaluation criteria the effects of the discharge are likely to be minor.

b Time co-incidence problems

Both the modelled and the background concentrations vary with time of day. In most cases the peak due to a point source emission does not occur at the same time as the background peak (which in many parts of New Zealand occurs during rush-hour traffic times or where wintertime domestic burning is carried out, during inversion layers that form over night). High background concentrations therefore almost always occur in calm to light wind conditions, when plumes from point sources may not reach the ground. On the other hand, point source peaks usually occur in:

(a) highly unstable daytime conditions
(b) in stable, light-wind night-time conditions or
(c) during the transition from night to morning, when fumigation may occur.

c Peak vs average

Should modelled peaks be added to measured peaks? Or averages to averages? Or peaks to averages? Each can give very different results. The most sensible approach is to add a peak (or 99.9 percentile) modelled result to an average background, since it is highly unlikely that the peaks in the two cases will ever be co-incident. However, if the peak background concentrations do occur under the same conditions as the peak concentrations from the discharge then the two peaks should be added together.

A study on how to add peak predicted concentrations to background values was recently undertaken by the UK Environment Agency (Environment Agency, 2000). The study concluded that simply adding peak model concentrations to background concentrations can result in severe overestimation of the source contribution, and that a more realistic method is to add twice the annual mean background concentration to the peak (or 99.9th percentile) modelled concentration. This method has not been reviewed or trialled in New Zealand, and it is not possible to comment on its relevance to the New Zealand situation.

Recommendation 66

When assessing the cumulative effects, use available background concentrations and account for the:

a) spatial co-incidence
b) time co-incidence
c) peak verses average concentrations
d) issues that may exist between the modelled and monitored (or estimated) background concentrations.

6.5 Assessment of effects

The final part in the process of deciding whether the model uncertainty is acceptable is to use the modelling result to assess some effect of the contaminant on people or the environment. Even when a lot is known about the effects, there are large uncertainties in the actual individual effect. Formaldehyde is a good example: some people are sensitive to quite low values, whereas others can easily tolerate concentrations 10 to 100 times higher. Which value should be chosen?

Recommendation 67

Before undertaking modelling and preparing an assessment of effects, consult the relevant environmental authority and check out the *Good Practice Guide for Assessing Discharges to Air* (currently under development by the Ministry) to determine:

a) the contaminants of greatest concern
b) the potential adverse effects that need to be assessed
c) the sensitivity of the receiving environment
d) the assessment criteria that will be used to assess the modelling results.

6.5.1 Evaluation criteria

There are a number of ways to assess the environmental and health effects of discharges to air once modelling results are available. The first step is evaluation against the national environmental standards. More information on how to do this will be included in the *Good Practice Guide for Assessing Discharges to Air* (currently under development by the Ministry). This new guide will cover:

- information required to undertake an assessment
- guidance on the level of assessment required depending on the scale and significance of the discharge
- guidance on when modelling is required
- interpretation of results against national environmental standards
- recommended evaluation criteria for pollutants not covered in the national environmental standards
- guidance on when a full health risk assessment is required.

6.6 Unresolved issues

Despite the vast amount of research that has been conducted on dispersion modelling and the fact that it is used hundreds of times a day all over the world, there are several issues that remain essentially unresolved. These include issues relating to missing data, calms, extreme weather, trends and synergistic effects.

6.6.1 Missing data

There are often missing data periods, in both emissions and meteorological data sets. Since most models will not tolerate missing data, various techniques are used to fill these holes for the purpose of getting the model to run at all. What if a critical period is missing? Say the peak emission rate, or a particularly awkward period of weather. When this is noticed, it can be accounted for in some way, although often it might not even be noticed.

Recommendation 68

Carefully review the model and all of the input data for potential occurrences of missing data.

This is the modelling 'reality check', and its value should not be underestimated.

6.6.2 Calms

When the wind speed drops below about 0.5 m/s, the wind direction becomes undefined and unresolvable, and the plume can end up going anywhere, or simply pooling. Unfortunately, these are exactly the circumstances which can lead to the highest ground-level concentrations but which cause the steady-state Gaussian equations to fail completely (wind speed appears on the bottom line of the equations, and cannot be zero). To handle this, the model forces a minimum wind speed of typically 0.5 m/s (it used to be 1 m/s, and in future it may be less). Puff models are a little better, and in theory allow for very light winds. Under these conditions the puffs are able to diffuse and grow without being advected. Fortunately, for most locations and most discharges, this is a rare circumstance.

Recommendation 69

If calms are identified as a potential concern, a more complete risk analysis should be completed. This analysis should at least consider the frequency and the potential consequences of calm conditions.

6.6.3 Extreme weather

With a one-year meteorological data set it is entirely conceivable that the worst-case meteorological conditions are not identified, and thus not modelled. This is a common criticism of modelling, and in many cases needs to be addressed with a specific study on the representativeness of the period of data used. This is done by comparing some statistics of the modelling data set, such as average wind speed, with those from the closest long-term climate station in order to assess the representativeness of that particular period.

Recommendation 70

The potential effects of extreme weather on pollutant dispersion should be identified.

The meteorological data set that is being used should be checked to ensure it contains conditions that allow for the effects of extreme weather to be assessed.

6.6.4 Trends

Similar comparisons to those outlined above should be made for long-terms trends such as climate change, land-use patterns, buildings, or even drifts in emission rates that could potentially alter the modelling results.

Recommendation 71

Modelling studies should identify and address any long-term trends that may affect the conclusions of that particular study (e.g. increasing background levels over time).

6.6.5 Synergistic effects

It is well known that some contaminants have worse effects in the presence of others than they do on their own. This is a very specialised subject, and not addressed by any current dispersion models, nor most common guidelines.

7 Glossary

If the term you are looking for is not included in this glossary, further terms can be found at the California Air Resources Board, Glossary of Air Pollution Terms web page (www.arb.ca.gov/html/gloss.htm).

Advection	Transport of pollutants by the wind
Airshed	An area, bounded by topographical features, within which airborne contaminants can be retained for an extended period
Algorithm	A mathematical process or set of rules used for calculation or problem-solving, which is usually undertaken by a computer
Assessment of environmental effects	A piece of expert advice submitted to regulators to support a claim that adverse effects will or will not occur as a result of an action, and usually developed in accordance with section 88 of the Resource Management Act 1991
Atmospheric chemistry	The chemical changes that gases and particulates undergo after they are discharged from a source
Atmospheric dispersion model	A mathematical representation of the physics governing the dispersion of pollutants in the atmosphere
Atmospheric stability	A measure of the propensity for vertical motion in the atmosphere
Building wakes	Strong turbulence and downward mixing caused by a negative pressure zone on the lee side of a building
Calm / stagnation	A period when wind speeds of less than 0.5 m/s persist
Cartesian grid	A co-ordinate system whose axes are straight lines intersecting at right angles
Causality	The relationship between cause and effect
Complex terrain	Terrain that contains features that cause deviations in direction and turbulence from larger-scale wind flows
Configuring a model	Setting the parameters within a model to perform the desired task
Convection	Vertical movement of air generated by surface heating
Convective boundary layer	The layer of the atmosphere containing convective air movements
Data assimilation	The use of observations to improve model results – commonly carried out in meteorological modelling
Default setting	The standard (sometimes recommended) operating value of a model parameter
Diagnostic wind model (DWM)	A model that extrapolates a limited amount of current wind data to a 3-D grid for the current time. It is the 'now' aspect, and makes the model 'diagnostic'.
Diffusion	Clean air mixing with contaminated air through the process of molecular motion. Diffusion is a very slow process compared to turbulent mixing.
Dispersion	The lowering of the concentration of pollutants by the combined processes of advection and diffusion
Dispersion coefficients	Variables that describe the lateral and vertical spread of a plume or a puff
Dry deposition	Removal of pollutants by deposition on the surface. Many different processes (including gravity) cause this effect.

Eddies	Small-scale turbulent disturbances contained within a larger air flow
Elevated receptors	Receptors that are on the ground but above the level at which the contaminants are released
Emission factors/models	A method used to calculate the amount of emissions that a particular source will release
Emission rates	The rate at which contaminants are discharged from a particular source
Emission temperature	The temperature of the gas stream that carries the contaminants from the source
Eulerian dispersion model	The pollution distribution is described by changing concentrations at discrete points on a fixed grid
Exit velocity	The velocity at which the exhaust gases leave a stack
Far field	Locations more than about 10 km from the source region
Flagpole receptors	Receptors that are located on structures above ground level
Fumigation	The process whereby pollutants held above an inversion layer are transferred back to ground level during the break-up of the inversion
Gaussian plume	A plume within which the pollutants are distributed vertically and horizontally in a Gaussian (or normal) manner about the plume centreline
Inversion	The situation where temperature increases with height; a highly stable condition in which vertical dispersion is suppressed and pollution is trapped
Katabatic flows	Downslope flow at night due to the air on the slope being cooler than the air at the same altitude away from the slope. The horizontal temperature gradient induces the downslope flow.
Lagrangian model	The pollution distribution is described by a set of discrete particles or puffs, which are labelled by their changing location (i.e. their trajectories are followed)
Macro-scale	Large spatial scale, 1000 km plus
Mechanical momentum	The upward (or otherwise) force a stream of gas exerts due to the velocity with which it leaves the point of discharge
Mesoscale	Medium spatial scale, 5 – 100 km
Micro-scale	Small spatial scale, less than 5 km
Mixing height	The height in the atmosphere to which pollutants released at the surface can be mixed by turbulent eddy motion
Model performance	A measure of a model's ability to reliably predict pollutant concentrations
Model sensitivity	The scale to which model predictions change when the value of a particular input parameter is changed
Model validation	The process used to demonstrate that a model produces reliable output
Modelling domain	The area over which the model is making predictions
Near field	The area close to the source, usually within a few km
Orographically driven flows	Winds driven by the relief of mountains and hills
Plume depletion	The removal of pollutants from a plume by gravity or chemical reaction
Plume rise	The height to which a plume rises above its release point due to its initial momentum and thermal buoyancy

Polar grid	A receptor grid defining a group of points located on a series of concentric circles, which are usually centred on the source
Prognostic model	A meteorological model which solves fully time-dependent equations, predicting the future from a known current state
Receptor	The location at which modelled concentrations need to be calculated
Radiosonde	Instruments suspended beneath a balloon to sense and relay temperature, humidity and pressure as the balloon ascends through the (whole) atmosphere
Screening	A model run that aims to calculate the highest concentration that might occur, but gives no information on the frequency or location of the event
Screening meteorological data	A synthetic data set that contains combinations of meteorological variables which include all possible atmospheric conditions (without saying how likely each would be to occur)
Sensitivity analysis	The process of establishing the effect of changing the value of an input variable on model output
Simple terrain	Terrain that will not influence larger-scale wind flows nor has receptors at a height greater than the release height of the pollutants
Slope flows	Air flows generated up or down hillsides by surface heating or cooling
Stability classification scheme	A simplified method of categorising the amount of turbulent mixing in the atmosphere
Stack-tip downwash	The small downward movement of a plume as it leaves a stack caused by a negative pressure zone on the lee side of the stack
Steady-state dispersion model	The Gaussian-plume; a mathematical solution to the dispersion equation, which is independent of time
Surface roughness length	A parameter needed in boundary calculations. Surface roughness increases the vertical mixing of an air stream due to enhanced mechanical turbulence generated as the air moves over surface features.
Thermal buoyancy	The buoyancy of a plume generated by the temperature difference between the exhaust gas and the ambient air
Turbulence	Small-scale (random) atmospheric motions that tend to mix pollutants through the air
Upper air data	Meteorological data that are collected above the height of a meteorological tower
Wet deposition	Removal of pollutants through scavenging by falling raindrops
Wind direction shear	A tendency for wind direction to turn with height
Wind field	The set of vectors that describe wind speed and direction conditions over a particular modelling domain at a particular hour
Wind speed profile	A measure of the rate at which wind speed increases with height above a surface

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Appendix A: Pasquill Turbulence Types

Table A1: Meteorological conditions defining Pasquill turbulence types*

Surface wind speed m/s	Daytime insolation			Night-time conditions**	
	Strong	Moderate	Slight	Thin overcast or > 4/8 low cloud	≤ 3/8 cloudiness
< 2	A	A–B	B		
2-3	A–B	B	C	E	F
3-4	B	B–C	C	D	E
4-6	C	C–D	D	D	D
> 6	C	C	D	D	D

Key: A: Extremely unstable; B: Moderately unstable; C: Slightly unstable; D: Neutral[#]; E: Slightly stable; F: Moderately stable.

Notes :

* From FA Gifford, 1976, Turbulent diffusion-typing schemes: A review, *Nuc. Saf* 17(1): 71.

\# Applicable to heavy overcast day or night.

** The degree of cloudiness is defined as that fraction of the sky above the local apparent horizon that is covered by clouds.

Appendix B: Site-specific Meteorological Data Sets

Table B1 contains a list of site-specific meteorological data sets that have been generated for use in New Zealand. This list is not definitive and is intended only to be a guide to the number and type of data sets that have been developed in New Zealand.

As noted in section 6 of this guide, the meteorological data are a critical input into any dispersion modelling study. It is therefore very important that the modeller is satisfied that any particular meteorological data set contains good-quality information and has been produced using standard/recommended methods. For this reason the data sets listed here have been classified into one of two categories.

Classification A

Meteorological data sets that have been:

- produced using recommended methods outlined in section 6
- subjected to peer review
- employed in a relatively large number of studies and resource consent applications.

Class A meteorological data sets are generally considered appropriate and robust for most applications in the relevant site.

Classification B

Meteorological data sets that have been:

- produced using a variety of methods, some standard some non-standard
- subject to limited or no peer review
- used for a small number of specialised applications.

The limitations of Class B meteorological data sets should be carefully considered before using them in a particular study. It may be helpful to justify your selection of the data set in the study's methodology.

Table B1: Site Specific Meteorological Data Sets Available

Location	Year	Model application	Classification	Contact
Auckland	1978	AUSPLUME	A	NIWA
Auckland	1996	AUSPLUME	A	NIWA
Christchurch	1979	AUSPLUME	A	ECAN
Christchurch	1991	AUSPLUME	A	ECAN
Christchurch	1997–98	AUSPLUME ISC3	A	ECAN
Auckland	1997 and 1999	CALPUFF AUSPLUME TAPM	B	NIWA
Auckland (Henderson)	1996	AUSPLUME ISC3	B	Terry Brady Consulting Ltd
Auckland (North Shore)	1998	AUSPLUME ISC3	B	Terry Brady Consulting Ltd
Awatoto	1995	AUSPLUME ISC3	B	Terry Brady Consulting Ltd
Blenheim	1997	AUSPLUME ISC3	B	Terry Brady Consulting Ltd
Christchurch	1997 and 1998	CALPUFF TAPM	B	NIWA
Christchurch (Hornby)	1998	AUSPLUME ISC3	B	Terry Brady Consulting Ltd
Gisborne	1995	AUSPLUME	B	NIWA
Hamilton	1997-1998	AUSPLUME ISC3	B	Terry Brady Consulting Ltd
Invercargill	1998	AUSPLUME	B	NIWA
Invercargill	1998-1999	AUSPLUME ISC3	B	Terry Brady Consulting Ltd
Kaitaia	1988	AUSPLUME	B	NIWA
Kaitaia	1988-1999	AUSPLUME ISC3	B	Terry Brady Consulting Ltd
Kawerau	1996-1997	CALPUFF	B	NIWA
Keri-Keri	1998	AUSPLUME ISC3	B	Terry Brady Consulting Ltd
Levin	1998	AUSPLUME ISC3	B	Terry Brady Consulting Ltd
Lower Hutt	1994-95	AUSPLUME	B	NIWA
Marsden Point	1989	AUSPLUME/ CDTMPLUS	B	NIWA
Napier	1999	CALPUFF AUSPLUME	B	NIWA
Nelson	2000	AUSPLUME CALPUFF	B	NIWA
Palmerston North	1996	AUSPLUME	B	NIWA

Location	Year	Model application	Classification	Contact
Palmerston North	2000	AUSPLUME ISC3	B	Terry Brady Consulting Ltd
New Plymouth	1996	AUSPLUME	B	NIWA
Paraparaumu	1997-1998	AUSPLUME ISC3	B	Terry Brady Consulting Ltd
Rotorua	1996	AUSPLUME	B	NIWA
Scott Base	1990	CALPUFF	B	NIWA
Stratford	2000	TAPM AUSPLUME	B	NIWA
Tauhara (Taupo)	1998	ASUPLUME	B	NIWA
Tauranga	1999	AUSPLUME ISC3	B	Terry Brady Consulting Ltd
Wanganui	2000	AUSPLUME ISC3	B	Terry Brady Consulting Ltd
Wellington	2000-2001	AUSPLUME CALPUFF	B	NIWA WRC
Wellington (Moa Point)	2000	CALPUFF AUSPLUME	B	NIWA
Westport	1998	AUSPLUME ISC3	B	Sinclair Knight Merz
Whitianga	1996	AUSPLUME ISC3	B	Terry Brady Consulting Ltd

Contacts:

Terry Brady Consulting Ltd	Terry Brady (09) 360-1080 terry@ebg.pl.net
ECAN	Tim Mallett (03) 365-3828 Tim.Mallett@ecan.govt.nz
NIWA	Clive Heydenrych (09) 375-4503 c.heydenrych@niwa.co.nz
WRC	Perry Davy (04) 384-5708 perry.davy@wrc.govt.nz
Sinclair Knight Merz	Philip Millichamp (04) 914-8422 PMillichamp@skm.co.nz

Appendix C: Estimation of Nitrogen Dioxide Concentrations from Modelled NO_x

C1 Introduction

Nitrogen oxides are emitted mainly in the form of nitric oxide (NO), but once released into the atmosphere are oxidised to the more toxic nitrogen dioxide (NO_2). The predominant short-term transformation process is the reaction of nitric oxide with ambient ozone to form nitrogen dioxide:

$$NO + O_3 \longrightarrow NO_2 + O_2$$

Since the reaction is a 1 to 1 transformation that does not affect total NO_x concentrations, the maximum extent of conversion of NO to NO_2 that can be expected in the emission plume is directly related to the maximum ambient concentration of ozone. Photo-dissociation of NO_2 to re-form NO and ozone decreases the concentrations of NO_2 to some degree, but is ignored here.

Ozone concentrations in air coming off the ocean are quite reproducible and show a seasonal variation, with the highest concentrations occurring during winter, at about 35 ppb at the Baring Head site. Summer concentrations are about 20 ppb. The maximum ozone concentration is sufficient to produce 72 $\mu g/m^3$ of nitrogen dioxide by oxidation of nitric oxide. This information provides the basis for a simple method for calculating generally conservative estimates of nitrogen dioxide concentrations from modelled NO_x concentrations.

C2 Relationship to the US EPA Ozone Limiting Method

This method of calculating nitrogen dioxide concentrations is related to the Ozone Limiting Method (OLM) available from the US EPA SCRAM website. The OLM describes only the modelling or calculation of annual average nitrogen dioxide concentrations, presumably because the US National Ambient Air Quality Standards include only an annual average standard of 100 $\mu g/m^3$ for nitrogen dioxide. However, the most sophisticated approach described under the OLM does use one-hour average modelling, together with one-hour average meteorological, ozone and nitrogen dioxide data, to calculate annual averages.

The OLM model requires simultaneously recorded one-hour average meteorological data, ozone and nitrogen dioxide concentrations extending over at least one year, with at least 90% valid data. Apart from the expense of obtaining such information at a single location, there are significant problems in locating the monitoring site relative to existing emission sources and the proposed new emission source. The US EPA guidance recommends two or more monitoring sites because of the perceived difficulty of accounting for scavenging of ozone by nitric oxide.

The method described here avoids the difficulties perceived in the OLM, and the ozone and NOx monitoring requirement, by recognising that for a small island country such as New Zealand, significant photochemical production of ozone is relatively rare at most locations and will seldom need to be taken into account when considering the local effects of NO_x emissions. The combination of this situation with the stable, but seasonally varying, concentrations of ozone in air moving onto New Zealand off the oceans means that realistic, but conservative, estimates of concentrations can be based on these ozone concentrations, the total NO_x

concentration at the site under consideration and the percentage of nitrogen dioxide in the NO_x in emissions affecting that site.

C3 The calculation methodology

For cumulative NO_x concentrations less than 80 µg/m^3 (expressed as nitrogen dioxide) all of the NO_x is considered to be present as nitrogen dioxide. The 80 µg/m^3 corresponds to 8 µg/m^3 of nitrogen dioxide resulting from a default percentage of 10% of nitrogen dioxide in emitted NO_x plus 72 µg/m^3 of nitrogen dioxide formed by oxidation of nitric oxide by ozone.

For cumulative NO_x concentrations above 80 µg/m^3, the nitrogen dioxide concentrations are calculated as follows:

$$[NO_2]_{cum\ max} = 72 + [NO_x]_{bkgrd\ tot} \times \%NO_{2\ bkgrd} + [NO_x]_{emiss} \times \%NO_{x\ emiss}$$

where:

- $[NO_2]_{cum\ max}$ is the maximum estimate of total cumulative NO_2 from both background NO_x and the additional emission under consideration
- $[NOx]_{bkgrd\ tot}$ is the total background NOx concentration in the receiving air
- $\%NO2_{bkgrd}$ is the percentage of nitrogen dioxide in the NOx emitted from the sources contributing to the background levels of NOx
- $[NOx]_{emiss}$ is the concentration of NOx at the receptor originating from the emission
- $\%NOx_{emiss}$ is the percentage of nitrogen dioxide in the NOx emitted from the source under consideration.

If either $\%NO_{2bkgrd}$ or $\%NOx_{emiss}$ are not known, the default percentage of 10% used in the OLM is probably the best (although often highly conservative) choice.

If the percentages of nitrogen dioxide in the emissions are not known, or happen to be 10%, the expression above simplifies to:

$$[NO_2]_{cum\ max} = 72 + [NOx]_{cum\ tot} \times 10\%$$

where:

- $[NOx]_{cum\ tot}$ is the cumulative total NOx concentration including both background NOx and the NOx concentration increment at the receptor resulting from the emission under consideration.

C4 Common situations resulting in conservative predictions

There are common situations where these calculations give substantial overestimates of nitrogen dioxide concentrations, including:

- during the day, when the photochemical equilibrium reverses the oxidation of nitric oxide by ozone to some degree
- during stable atmospheric conditions, particularly at night, when both nitrogen dioxide and ozone are removed by reaction with vegetation and other surfaces.

C5 Validation against monitoring data

Use of this method to calculate nitrogen dioxide concentrations from NOx concentrations measured at several monitoring sites in both Auckland and Christchurch shows that taking the percentage of nitrogen dioxide in NOx emissions contributing to the measured concentrations as 10% is highly conservative and that 5% still predicts nitrogen dioxide concentrations higher than any reliable measured concentrations. This may reflect the combined effect of the true percentage of nitrogen dioxide in NOx emissions being less than 10%, together with scavenging of both nitrogen dioxide and ozone by vegetation, plus the photochemical equilibrium.

C6 Caution re application of the method to some types of locations

The Khyber Pass site in Auckland is unique among New Zealand NOx monitoring sites in that nitrogen dioxide concentrations measured there quite frequently exceed the predictions using this method. After 7 pm and before 7 am, there are only a few hourly averages during the year when the measured nitrogen dioxide concentrations exceed those predicted using 10% as the percentage of nitrogen dioxide in NOx emissions, and essentially no measured concentrations exceed those predicted using 15%. However, during the remainder of the day, there are a considerable number of measured concentrations that exceed those predicted using 15% as the percentage of nitrogen dioxide in NOx emissions. This is in marked contrast to both the Penrose and Takapuna monitoring sites, both of which are dominated by traffic emissions, as is the Khyber Pass site, but which show few if any measured concentrations exceeding those calculated using 5% of nitrogen dioxide in NOx emissions.

The frequent, unusually high nitrogen dioxide concentrations at the Khyber Pass site may be associated with some of the following features of the site:

- the kerbside location alongside an uphill queue for traffic lights, with uphill exits in all directions
- the absence of any vegetation between the location of the emissions and the monitoring intake
- the relatively confined nature of the location, which may mean that relatively high concentrations of both reactive organic compounds and NOx from vehicle emissions may move away only slowly, so that there may be the possibility of photochemical reactions (this is consistent with most of the unexpectedly high nitrogen dioxide concentrations occurring during the day)
- the proximity of the site to the busiest section of the northern motorway, which may also contribute to relatively long residence times of high concentrations of reactive organic compounds and NOx in the area
- the relatively high proportion of diesel vehicles among the traffic flow, which may emit high percentages of nitrogen dioxide in NOx emissions at idle, immediately adjacent to the monitoring intake, while waiting for the traffic lights.

The calculation method described here should be used only with great caution at locations where NOx concentrations originate predominantly from vehicle emissions and which share some of the other features described above for the Khyber Pass site. Ideally, some monitoring data should be obtained to determine whether unexpectedly high concentrations occur at these locations.

Appendix D: Sources of Helpful Information

Source	Provider or publisher	Material	Website or author
Technology Transfer Network TTNWeb	Office of Air Quality Planing and Standards (US EPA)	Collection of related Web sites containing information about many areas of air pollution science, technology, regulation, measurement and prevention.	http://www.epa.gov/ttn/direct.html To search the TNN Web: http://www.epa.gov/ttn/ttn_search.html
Clearinghouse for Inventories and Emission Factors (CHIEF)	US EPA	Emission factor and inventory information, tools and software, publications, conference proceedings, related sites	http://www.epa.gov/ttn/chief/
Support Centre for Regulatory Air Models (SCRAM)	US EPA	Modellers forums, FAQs, model code and support, conference proceedings, related sites	http://www.epa.gov/ttn/scram/
Modelling Helpdesk	Casella-Stanger and Department for Food Environmental and Rural Affairs (DEFRA) UK	FAQs, toolkits and reports	http://www.casellastanger.com/JointProjects/DEFRA-Home.asp?jointprojectid=7
Air Quality, Emissions, and Modelling	California Air Resources Board	Emissions inventories and air quality models, and glossary of terms	http://www.arb.ca.gov/html/aqe&m.htm Glossary of terms found at: http://www.arb.ca.gov/html/gloss.htm
Air Quality Modelling Forum	Western Region Air Partnership (WRAP) (US)	WRAP aims to develop data, tools, and policies needed to improve air quality	http://www.wrapair.org/forums/aqmf/index.html
Model Documentation System	European Topic Centre on Air and Climate Change	Aims to provide guidance to any model user in the selection of the most appropriate model for a specific application	http://air-climate.eionet.eu.int/databases/ mds.html
TAPM	CSIRO	Description, documentation, availability and support for TAPM	http://www.dar.csiro.au/tapm/
CALMET-CALPUFF	Earthtech	Description, documentation, availability and support for CALMET and CALPUFF	http://www.src.com/calpuff/calpuff1.htm
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes	National Environmental Research Institute Denmark	Workshop and conference proceedings, model validation kit, tools for dispersion modelling	http://www.harmo.org/
Open Directory	Open Project Directory	Comprehensive and interesting list of air quality modelling resources	http://dmoz.org/Science/Environment/Air_Quality/Air_Dispersion_Modeling/Software/
National Climate Database	NIWA	New Zealand's national repository of high-quality climate data	http://www.niwa.co.nz/services/clidb
Terralink	Terralink International	Provider of land information	http://www.terralink.co.nz/

Source	Provider or publisher	Material	Website or author
Handbook on Atmospheric Diffusion	Technical Information Center, US Department of Energy	Textbook	Hanna SR, Briggs GA, Hosker RP, 1982. Prepared for the Office of Health and Environmental Research, Office of Energy Research, US Department of Energy Document number DOE/TIC-11223 (DE82002045)
Fundamentals of Atmospheric Modelling	Cambridge University Press, Cambridge UK.	Textbook	Jacobson MZ, 1999 ISBN 0521637171
Workbook of Atmospheric Dispersion Estimates	National Technical Information Service, Springfield VA, USA	Textbook	Turner DB, 1970
Fundamentals of Stack Gas Dispersion (Ed 3)	Milton R Beychock, 2233 Martin Street, Unit 205, Irvine, CA92612	Textbook	Beychock MR, 1994 ISBN 0-9644588-0-2
Turbulence and Diffusion in the Atmosphere, Lectures in Environmental Sciences	Springer	Textbook	Blackadar AK, 1996 ISBN 3-540-61406-0
Atmospheric Dispersion Modelling Compliance Guide	McGraw-Hill	Textbook	Schnelle KB, Dey PR, 2000 ISBN 0-07-058065-0
Modelling Special Interest Group (ModSIG)	Clean Air Society of Australia and New Zealand	The primary purpose of ModSIG is to bring together CASANZ members who have an interest in the development and/or application of air quality models	http://www.casanz.org.au/