Guidelines for the Preparation of Dispersion Modelling Assessments for Compliance with Regulatory Requirements – an Update to the 1995 Royal Meteorological Society Guidance

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EXECUTIVE SUMMARY

The Atmospheric Dispersion Modelling Liaison Committee (ADMLC) feels that some applications of atmospheric dispersion models are inadequate, and that this may reflect a lack of appropriate guidance/training in Atmospheric Dispersion Modelling. ADMLC considers that publication of up to date guidance on Dispersion Modelling may be one way to facilitate possible improvement in applications although this cannot be a replacement for proper training.

The Royal Meteorological Society (RMetS) produced a set of guidelines in 1995 which were intended to promote the use of best practice in the use of mathematical models of atmospheric dispersion, emphasising the principle of fitness for purpose in the selection of modelling procedures, and the importance of effective communication in the documentation of reported results. The underlying objectives are to ensure the efficient use of resources, especially in the context of assessments conducted for purposes of demonstrating compliance with regulatory obligations.

The RMetS guidelines set down general principles of good practice for the design, execution and communication of modelling studies, focussing on broad principles which apply across a wide range of environmental modelling situations.

They did not try to give situation-specific technical advice, e.g. how to model a dense gas spill, or which plume rise formula to use. Instead, they tried to identify and expound certain principles of good practice which apply to many modelling situations.

ADMLC feels that sufficient time has passed since the RMetS guidelines were prepared, and that modelling techniques have evolved over the intervening period, that there is merit in preparing further guidelines which will update, extend and complement, rather than replace, the existing ones. This guidance is intended to improve the robustness of assessments by providing advice on addressing the scope of the assessment, selecting and justifying an appropriate model and effective communication in the documentation of reported results. It follows the style of the original guidelines by addressing general principles rather than providing advice on the most appropriate methods of modelling particular situations.

It follows the same structure and uses the same section headings as the original RMetS guidance. This guidance is intended as an update of the original guidance; however, much of the text of the original document is included here and to that extent this document can be considered as replacing the earlier guidance.

The RMetS has agreed to the preparation of this revised guidance.

CONTENTS

1 INTRODUCTION

Setting out the aim and objectives of this Updated Guidance and its structure.

1.1 Why new guidance

In 1995 the Royal Meteorological Society (RMetS) published guidance on the justification of choice and use of atmospheric dispersion models and the communication and reporting of results of using such models (RMetS 1995) (hereon referred to as the RMetS 1995 guidance). In 2000, the Environment Agency (EA) published its policy on the choice of air dispersion models (Environment Agency 2000; see Box 1) making reference to the RMetS 1995 guidance.

This Updated Guidance has been produced with the aim of extending the RMetS 1995 guidance in light of the EA's policy to improve the robustness of atmospheric dispersion modelling assessments. An important part of the update was to obtain comments from the modelling community on the scope and contents of the document. An outline of the report was placed on the ADMLC web site for comment. A draft version of the final guidance was subsequently placed on the ADMLC web site for comment. This final version responds to the comments that were received on that draft.

This guidance primarily relates to air quality assessments undertaken for the purposes of an environmental impact assessment as part of a planning application in accordance with the EIA Regulations, or for the purposes of securing a Pollution Prevention and Control permit in accordance with the PPC Regulations 2003. This guidance may also assist in providing guidance on assessments as part of local air quality management and other applications. The guidance was written primarily for applications relating to controlled releases, but may also assist in applications relating to incident investigation, emergency planning and emergency response. It provides specific guidance on:

- determining the scope of assessment
- model selection
- addressing sensitivity, uncertainty and variability
- communication.

This Updated Guidance should be considered as an extension to the RMetS 1995 guidance.

BOX 1 – ENVIRONMENT AGENCY POLICY EAS/2007/1/1

Choice of Air Dispersion Models

The Environment Agency does not favour or prescribe the use of any particular model. It is left to the operators/applicants to justify their choice of models (including the version). However, the chosen model (and specific version) has to be fit for purpose and based on established scientific principles. It also needs to have been validated and independently reviewed. For transparency reasons, the Agency expects full technical specifications, validation and review documents of the chosen model (and the specific version) to be publicly available. The Royal Meteorological Society (1995) has provided guidance on the justification of choice and use of models.

Environment Agency, 13 March 2000

1.2 How the Updated Guidance is structured

To assist the reader, this Updated Guidance has been laid out as follows:

- The same structure as for the RMetS 1995 guidance has been adopted.
- Each section begins with an overview in italics, taken from the Executive Summary of the RMetS 1995 guidance. This text is included here by agreement with the Royal Meteorological Society.
- The relevant RMetS 1995 guidance is quoted in full in a text box, with subsequent text in the main body of text representing the Updated Guidance.
- A full list of references of available guidance and relevant literature is included for completeness.

2 STATEMENT OF CONTEXT AND OBJECTIVES

To explain the situation being modelled and the purpose of the dispersion calculations, giving a clear account of the relationship between the objectives and the modelling procedures adopted to achieve them.

BOX 2 - STATEMENT OF CONTEXT AND OBJECTIVES

The documentation should include a clear statement of the context and objectives of the exercise, enabling the reader to form a proper understanding of the purpose of the study. Such a statement should describe the particular circumstances being modelled, identify the key issues and impacts of concern, specify the salient features of the regulatory requirement that the assessment is designed to address, and specify in some detail the objectives of the calculations in terms of receptors, locations and types of exposure, and the features of the exposure that are associated with various levels of impact. Overall, the statement should provide a definition of the scope of the exercise such that the stated objectives are related in a clear manner to the modelling procedures adopted.

RMetS 1995 guidance.

2.1 The scope of the assessment

As for all assessment reports, the aims and objectives should be clearly defined from the outset. In most circumstances an air quality assessment should include the following:

a A general description of the situation being assessed, whether a proposed or existing development, and the reasons for the assessment with reference to legislation as appropriate. Since the original guidelines were prepared, there have been a number of developments such as new air quality directives and strategies, which should be taken into account in specifying the appropriate legislation.

b Definition of operating scenarios, and the years covered by the assessment.

c Identification of key pollutants, relevant emission rates and limits and ambient air quality criteria (all of which may change depending on the scenario and assessment year).

d Description of underlying land cover (urban, agriculture, water, etcetera) and land use, identifying local receptors and sources of air pollution. Note that the EA has issued guidance on the distance criteria for receptors near to landfill and PPC application sites.

e Review of available ambient monitoring data (including projections for relevant assessment years) within the study area and from background sites upwind of the site being assessed.

f Justification for selection of representative meteorological data.

g Description of local building dimensions. For industrial sources this should include all buildings of height >= about a quarter of the height of stack or within a distance of 5L from the stack, where L is the lesser of the building height and maximum cross wind width. Individual building dimensions are not critical for road traffic assessments although due consideration should be given to the surface roughness length and street canyons.

h Description of local topographical features, including coastlines. Features within the model domain, such as hill heights greater than 50% of the stack height or slopes greater than 10% should be included.

i Justification for model selection, with particular reference to local building dimensions and topographical features. Note that the modelling of the effects of buildings and complex terrain in some models can be limited. This should demonstrate that the model chosen is appropriate for the type of buildings and/or terrain in the area being considered.

j Description and justification of how atmospheric chemistry is modelled.

k Description of how emissions data were compiled, including source of traffic data, continuous emissions monitoring data or process physico-chemical stoichiometric calculations.

l Running the model, including sensitivity analyses, to determine optimum stack height.

m Running the model, including sensitivity analyses, to determine compliance with relevant ambient air quality criteria.

n Presentation of results.

o Conclusions and recommendations.

Providing a detailed step by step description of the assessment method can assist in ensuring a clear understanding between the developer / applicant and the regulator and between the modeller and client / manager.

As with any assessment, the first step is to determine the likely scale and magnitude of the impact and hence, details of the assessment required. This can be achieved by comparing the additional atmospheric emissions with relevant limits or existing emissions.

In any circumstance it is good practice to secure prior agreement on the exact scope and limit of the air quality assessment with the relevant regulator. Defining the scope requires a clear understanding of the purpose of the assessment, its objectives and expected audience. This may be achieved by a face to face meeting in conjunction with a site visit followed up with a confirmatory letter, or by submission of a detailed assessment methodology for review and agreement,. The EA has published appropriate guidance to assist in making pre-application meetings as efficient as possible.

2.2 The importance of a site visit

All environmental modelling studies require the application of an idealised set of assumptions to describe environmental processes. A site visit not only allows the modeller to appreciate the specific environment being considered, particularly in terms of local buildings, land use and topography, but also to check for the presence of local sources of air pollution and sensitive receptors.

The modeller should be aware that the reader of the Report may not be familiar with the site and is reliant on sufficient information to be provided to appreciate how the assessment was undertaken, particularly in terms of how the model was set up to reflect local conditions.

The site description should make reference to the site visit and the inclusion of photographs, appropriate mapping and satellite imagery is recommended. This can assist the reader in understanding the scope and limitations of the assessment and the specific assumptions made.

3 CHOICE OF MODELLING PROCEDURE

To demonstrate the fitness for purpose of the modelling procedure.

BOX 3 – JUSTIFICATION OF CHOICE OF MODELLING PROCEDURE

The type of modelling procedure chosen should be described and justified in relation to the objectives. This should include consideration of criteria for the neglect or inclusion of factors that may determine the type of model that is appropriate. It may be necessary to consider, for example, the neglect or inclusion of non-passive dispersion behaviour, the influence of topography, surface conditions, and the presence of buildings on dispersion and source behaviour, the influence of coastal meteorology, and whether the setting is urban or rural. Consideration of the suitability of a model will need to be related to the specific characteristics of the site of interest. The fact that a particular mechanism is not included in a model that is available, or that it would be difficult or expensive to address, should not be regarded as an adequate criterion for exclusion from the assessment if there is a case for its inclusion on technical grounds. The guiding principle in the justification of the chosen procedures is the demonstration of fitness for purpose. Although in many cases there will be a need to use software implementations of models, there may also be aspects where the use of scoping calculations is all that is needed. For example, where such calculations reliably show that the upper limit of a numerical quantity is so far below an appropriate reference level of concern that more detailed estimation is not merited, it would be a waste of resources to apply more involved methods.*

RMetS 1995 guidance.

* Note that developments since the original guidelines were prepared mean that surface roughness length is used in advanced dispersion models in preference to this simplistic description.

3.1 Screening

Although this guidance has been written assuming a detailed modelling assessment is required, there are circumstances when a screening exercise may be sufficient to demonstrate compliance with relevant emission limits and ambient air quality criteria. The Department for Environment, Food and Rural Affairs (Defra) provides advice on how to approach screening for the various pollutants (see the Defra web site http://laqm.defra.gov.uk/documents/LAQM-TG-(09)-Dec-12.pdf or more specifically http://laqm.defra.gov.uk/technical-guidance/index.html?d=Chapter5), and this is supplemented by guidance from the EA (Environment Agency 2002). In all cases where screening alone is thought to be sufficient, an agreement should be reached with the relevant regulatory body that this is accepted.

3.2 Selection procedure

The choice of which modelling procedure to adopt for a particular assessment is dependent upon several factors, primarily:

a Can the model adequately describe the circumstances being assessed?
b Is the model output sufficient for the assessment?

Resource or time constraints should not influence the choice of model, but the work in preparing the assessment should be planned in such a way that these are avoided. The procedure adopted should be related to the predicted or perceived environmental risk.

Clearly the modelling procedure needs to describe both the source of atmospheric pollutants and all relevant influences upon dispersion through the atmosphere. The selection of a model and how it is used needs to consider the following aspects:

a The number of sources being considered
b Averaging times and relevant percentiles
c Building wake effects
d Complex topography, including features such as coastlines
e Atmospheric chemistry
f Inclusion of background air quality data
g Validation of the model with respect to the particular conditions being modelled
h Model run time.

Furthermore, the model has to generate results in the correct form to allow for interpretation and evaluation with reference to relevant assessment criteria.

An example checklist is provided in Table 1 to assist the modeller in determining these issues.

Table 1 – Checklist for Model Selection

Model Effect	Relevant to this assessment? (Y/N)	Adequately included in the model with sufficient validation? (Y/N)
Source type (point, line, area, volume)		
Number of sources		
Source description		
Averaging period		
Building wake		
Street canyons		
Complex topography		
Meteorology		
Receptor grid density		
Coastal effects		
Fumigation		
Atmospheric chemistry		
Precipitation		
Deposition		
Background contributions		
Interface with other software (e.g. GIS)		

4 USE OF SOFTWARE

To provide a fully documented account of the details of the model and its conversion into valid software.

BOX 4 – USE OF SOFTWARE IMPLEMENTATIONS OF MODELLING PROCEDURES

In order that the recipient of the report on the exercise can assess the appropriateness of the models used it is essential that full documentation of the modelling procedures should be available. Preferably this should be in the public domain, but it is recognised that this may not always be practicable for a number of reasons, such as the need to protect the commercial investment in software development. In such cases an acceptable alternative would be for the relevant documentation to be made available to parties with a legitimate interest. The documentation should include a general account of the model, separate from the report of the particular application. It will often be helpful to include copies of these general supporting documents with the account of the particular exercise.

Where computational methods are employed, a minimum level of documentation of the model itself should include i) an account of the mechanisms that are addressed, together with a description of the mathematical relationships by which these mechanisms are represented, ii) a description of how the mathematical model has been converted to a form suitable for incorporation into software, including the algorithms used, the structure of the computer code, and a summary of the tests that the software has undergone, and iii) a user's guide which includes detailed instructions on how the model is to be used, *and examples of model runs showing both input data and sets of results. Data files used in the modelling, both for specific properties of substances, and for modelling parameters such as dispersion coefficients, should be documented. It is strongly recommended that models for which such documentation is not available should not be used for the types of exercises discussed here.*

RMetS 1995 guidance.

4.1 Modelling procedures

The RMetS 1995 guidance includes issues relating to model development. In practice, most dispersion modelling studies are undertaken using proprietary software. The necessary model documentation should be available and its source should be included in reporting the results of a modelling assessment. The availability of adequate documentation of the model could be regarded as one of the tests of model suitability.

The model user is recommended to consider the whole modelling assessment process and not just the dispersion model itself. The following stages in the modelling assessment may all include mathematical procedures and software implementation which may be distinct from the dispersion model:

- **Emissions data** – whether derived from manufacturer's guarantees, thermodynamic combustion calculations, national fleet emissions and activity data, etcetera.
- **Topographical data** – whether supplied from a cartographer to an agreed format and density, reprocessed to some different density, or derived from raw data.
- **Meteorological data** – whether derived from internationally accepted weather observation techniques or from Numerical Weather Predictions (NWP) and specifying any subsequent pre-processing.
- **Percentile post processing** – use of spreadsheets or procedures outside the dispersion model to calculate percentiles or other summary statistics should be documented, including checking procedures.
- **Contouring** – the interpolation procedures used for constructing contours should be clearly documented. This element of a modelling assessment can be a significant source of (undocumented) error.

The model user should consider which elements of the dispersion model are being used and whether sufficient documentation is available to demonstrate that the software accurately reflects the mathematical procedures being included in the assessment. Where any mathematical procedures are included that are separate from the dispersion model, sufficient reference to adequate documentation should be provided as part of the Report.

5 INPUT DATA

To show how the data requirements of the model have been met, and to explore the implications on the assessment in cases where there are deficiencies in the available data.

BOX 5 – INPUT DATA

The models used, of whatever type, will require input data of various categories. UK practice has been characterised by a tendency to accept that site-specific data are often unavailable. It is recommended that a more pro-active approach needs to be adopted, particularly where the planning timescales of projects are sufficiently long to permit this. For some important factors direct measurements are always to be preferred to estimates of those factors derived from other measured quantities. Where dispersion will be affected by the local terrain, for example in areas close to coasts or where there are significant topographical features, it is recommended that measurements of relevant quantities should be made at the site for a reasonable period, such as one year. These measurements can then be related to data obtained over longer periods at the most representative nearby site having such records. Where a decision is made, for reasons of economy or time, not to collect on-site data, information must nonetheless be provided in order that the assessment can proceed. In such cases the assessment may make use of meteorological data for nearby sites that are representative of the region, and as representative as possible of the site in question, with a view to examining how these differing inputs would affect the overall decision. Where such an approach is adopted careful consideration needs to be given to the question of the degree to which data from another site are representative of the location for which data are lacking. Geographic proximity alone is not a sufficient criterion in this respect, as differences in terrain may well make the comparison invalid. Sources of data should be specified in detail, and where data that are used are of such a type that it is necessary to select those to be used from a number of candidate options, the selection made should be justified. Assessments should examine the full range of climatology, including extremes where these are important to the nature of the impact, as well as more typical conditions. An account should be given in all cases of the quality and representativeness of the data used, so that the limitations imposed by the availability of suitable data are fully exposed.

RMetS 1995 guidance.

5.1 Updated Guidance

With further contractions in the UK network of weather stations the use of representative meteorological data is of more concern than in 1995. However, the principle of assessing how representative input data are is common to all parameters.

Compiling a list of all model input data is recommended, with consideration given to the likely range in values under typical and atypical conditions. This can then be used as the basis for uncertainty analyses, as described in Section 7.

6 COMMUNICATION

To ensure that the findings of the exercise are successfully communicated.

BOX 6 – PRESENTATION OF RESULTS AND CONCLUSIONS

Presentation of results should make good use of quantitatively labelled graphical summaries (such as maps overlaid with concentration contour plots) wherever possible, and should not rely solely on tables of numbers. In any case, all numerical quantities should be clearly labelled with the appropriate units. Conclusions should be expressed in a manner that bears a clear relationship to the stated objectives and to the results obtained from the modelling procedure. All conclusions should be made explicit, and should not have to be inferred by the reader.

RMetS 1995 guidance.

To ensure that best use is made of the opportunity to express results in quantitative terms.

BOX 7 – EXPLICIT QUANTIFICATION

Results should always be fully quoted as numerical values in any discussion of their significance. Inferences and conclusions should be substantiated by explicit reference to the numerical quantities on which the argument is based; the discussion should not contain unsubstantiated assertions. For example, if it is argued that a quantity is of negligible importance in relation to some reference level, both should be explicitly quoted so that the quantitative interpretation of negligibility is clearly expressed. Quantitative descriptions should be used wherever possible in order to avoid ambiguity. For example, different parameter values may well be required for winds blowing from the sea to the land as compared with the reverse case. The wind directions for which this is the case should be specified, since the meaning of on shore and off shore directions will only be unambiguous in the idealised case of the long straight coast line.

RMetS 1995 guidance.

6.1 Introduction

The presentation of results and any conclusions drawn from them is the key element of reporting an assessment, as these are the aspects most likely to be read and scrutinised. In presenting results, the report author should consider the following:

a Is there a clear link between the scope and objectives of the modelling study and the results presented?

b Is there clear reference to relevant assessment criteria, such as air quality criteria, odour requirements, etc.

c Is good use made of tables, graphs and contour plots?

d Are the results comprehensive with sufficient reference to model sensitivity and robustness?

An air quality assessment can generate significant quantities of results and analysis. A key skill in presenting the results is to include only those that are relevant to the study objectives and at the same time demonstrate the robustness of assessment.

6.2 Tabulation of data

Tables should be presented as stand alone summaries of results. The reader should be able to view the table and draw conclusions from the results presented. The Table should include, for example, any relevant air quality criteria, background air quality data and the model results for direct evaluation.

6.3 Graphical presentation

The use of graphs can assist in the interpretation and presentation of results. Axes should be clearly labelled.

6.4 Contour Plots

The use of contour plots is a common means of illustrating the scale and magnitude of an air quality impact. Plotting the contours onto a suitable base plan (e.g. Ordnance Survey) assists in this, particularly when key features, such as sensitive receptors, terrain features and other sources of air pollution are identified. Contour plots should include a scale and northing, with the plot extending sufficiently to include full contours.

7 SENSITIVITY, UNCERTAINTY AND VARIABILITY

To expose how the results depend on choices and assumptions made in respect of variables whose values may be debatable, and to ensure that these issues are addressed in respect of uncertainties in model parameters, the inherent variability of dispersion behaviour and the variations that are likely to be displayed between the results of one model and another.

BOX 8 – SENSITIVITY ANALYSIS

Model sensitivity to user selected variables may be important in determining the results of the assessment. Where the assessment depends on the results obtained using choices of variables that may be debatable, sensitivity analysis should be conducted, and the results expressed. A summary of the cases considered in the analysis, presented in *the form of a table or matrix of parameters examined and the associated effects on salient outputs, will often provide an effective means of communicating the results. Unsubstantiated assertions as to the insensitivity of the results to certain factors should not be made, but instead the argument should be demonstrated by reference to quantitative examples.*

RMetS 1995 guidance.

BOX 9 – UNCERTAINTY AND VARIABILITY

The estimation of atmospheric dispersion behaviour is subject to numerous sources of uncertainty. These include ones arising from the approximation represented by the model itself, those attributable to the range of choice available in relation to the user defined parameters, and the incompleteness of our knowledge of dispersion behaviour. Additionally, the dispersion process is inherently variable, so that the exposures resulting from a sequence of release episodes occurring in conditions that are apparently identical in terms of observed meteorology will inevitably differ. Since models produce concentration estimates that are averaged in various ways, it is to be expected that these averaged quantities will differ from those observed in a single dispersion episode. The model user should give some estimate of the uncertainty that attaches to the results, and should address the issue of variability. If this is done much of the apparent disagreement between models, and between measured values and those estimated by models, may be encompassed within the ranges of uncertainty. Failure to address these issues is likely to result in loss of credibility in the use of dispersion modelling as an aid in decision-making where, for example, unresolved differences consume a disproportionate amount of time in a public inquiry. Modellers and model users have a responsibility to ensure that these issues are addressed so that they do not become sources of confusion in the decision making process. Where this happens the result is often that the dispersion modelling exercise as a whole is discredited, and the potential usefulness of the information is lost.

RMetS 1995 guidance.

7.1 Introduction

A typical dispersion model may require the user to input some twenty to thirty parameters in addition to meteorological data, which may include between five and ten parameters for each unit of time modelled. A prime objective of all modelling studies should be to demonstrate a high degree of robustness in assessment. This requires an understanding of the *sensitivity* of the model to key input parameters which, in turn, may be used to address the inherent *uncertainty* in model parameters and *variability* in dispersion behaviour. Some degree of variation is also expected when using different models. This is addressed in Section 8.4. Definitions of sensitivity, uncertainty and variability are included in Table 2.

Table 2 – Sensitivity, Uncertainty and Variability

	Definition	Statistic	Working
Sensitivity (S)	The differential of model output by model input	$S = \frac{\delta y}{\delta x}$	An assessment may be considered sensitive to a model input parameter if varying the parameter value within a given range alters the conclusions of the assessment (e.g. an air quality criterion is breached or not).
Uncertainty (U)	The change of model output for a plausible change in model input	$S = \frac{\delta y}{\delta x} \cdot \delta x$	Uncertainty may be expressed by reporting a range of model results rather than a single number. For example, by running the model several times for given ranges of key input parameters, then reporting the mean ±twice the standard deviation.
Variability (V)	That which cannot be reduced by further experiment.		Some degree of variability is implicit in attempting to use a model of a natural system. For example, year on year variations in meteorology will affect the model output. In this case, variability can be expressed by using several years of meteorological data and reporting the mean ±twice the standard deviation.

7.2 Key input parameters

The atmospheric dispersion model will be sensitive to the following key parameters:

a **Emission characteristics –** including mass emission rates, stack height, efflux velocity and efflux temperature. For road schemes, the number and length of straight line links used to model a curved road can be critical for near source receptors.

b **Meteorology –** experience suggests dispersion models are sensitive to inter-year variability in meteorology, particularly for elevated releases[†]. In some circumstances wholly representative data are not available and data from two or more weather stations need to be included in the assessment.

c **Atmospheric chemistry** Atmospheric chemistry can significantly influence the model results. Speeds of some chemical reactions are affected by atmospheric conditions, and this may influence the choice of meteorological data or the number of years of data considered.[‡]

[†] Environment Agency guidance suggests the use of five years of hourly sequential data. The financial difficulties experienced by Local Authorities in obtaining and using data for more than one year forced a pragmatic recommendation of using data for only one year in the Defra guidance. This will be revised when the guidance documents are reviewed in 2007. It is suggested here that more than one year should be considered to give an indication of the extent of inter-annual variation.
[‡] Carruthers et al (2003) suggests that the method of modelling atmospheric chemistry can be at least as significant as inter year variability in meteorological data.

d **Terrain –** experience suggests terrain features are significant for elevated releases but not generally for surface level releases such as road schemes, where the effects are usually within 10 to 20 m of the kerb, unless cuttings and embankments have an effect on the dispersion. Terrain should be included if the change in altitude (above or below the release point) or the slope could have an impact on the model predictions. The description of terrain effects in dispersion models is limited and, in conjunction with surface roughness, should be considered in some depth as part of the sensitivity analysis.

e **Buildings –** Buildings greater than one quarter of the height of an elevated release and within 5L of the source will have some effect on dispersion. However, the description of building wake effects in dispersion models is extremely limited. It is recommended that a simple study should be conducted to understand the sensitivity of the model to a particular building. This might involve, for example, calculating the maximum short-term contribution from a source for different building heights, or for different ratios of building width to length, depending on the assumptions made in approximating the physical structure by a simple building shape. Street canyon effects caused by buildings can also be significant but are also described in a limited way by dispersion models.

f **Coastal effects –** if applicable, should be included as part of the sensitivity analysis.

g **Receptor spacings –** the number of receptors included in the model run is a function of the density of receptors and the spatial extent of a model domain. An increase in the number of receptors will increase model run time. As the air quality impact of road traffic emissions is typically within 10-20 m of a roadside, the spacing or placement of receptors relative to the road link being modelled is critical.

The sensitivity of the model to any combination of the above input parameters should also be considered and accounted for.

7.3 Uncertainty

Uncertainty can be expressed as the likelihood that a value lies within a given range. An appropriate degree of uncertainty could be the range within which 97.5 % of the values are found, which is equivalent to the mean ± twice the standard deviation. In this instance, the estimated range of uncertainty is expressed as twice the standard deviation divided by the mean.

In practice, an indication of uncertainty can be considered in two ways, after first using observed data, experience and/or judgement to define the likely range that an input parameter will lie within:

Either:

undertake a Monte Carlo analysis to define the mean and standard deviation. These values are then used to determine the sensitivity of the model to this parameter.

Or:

use a Chi Square test to select combinations of minimum or maximum values for individual input data, and to determine the mean and standard deviations from the resultant model runs.

7.4 Variability

In most circumstances inter-year variations in meteorological inputs will significantly influence variability in dispersion. The same method used to express uncertainty can be used to consider the effect of variability in meteorological data, e.g. determine the five year mean ± twice the standard deviation.

8 QUALITY ASSURANCE

To demonstrate that the model used has been subjected to an evaluation procedure establishing its suitability for a specified range of tasks.

BOX 10 –QUALITY ASSURANCE

Quality assurance of models depends largely on the model evaluation procedures referred to earlier. Evaluation of a model includes the distinct procedures of verification, validation, and (where appropriate) scientific assessment. At the very least, a computer model should not be used unless it has been verified, that is, shown by a detailed examination to be a true version of the mathematical model which it incorporates. Such verification should be carried out independently of the personnel who constructed the model. Model verification is a painstaking task of checking that the coding faithfully reproduces the mathematical model approximations incorporated in the algorithms, and as such is one of the easier parts of the evaluation procedure. Additionally, a model should be subjected to a process of validation, that is, its results should be compared with an independent dataset, and the accuracy and reliability of the model assessed. This is a much more difficult task, and the degree to which a model can be said to be validated, and in what respects, is more open to debate. It is recommended that users should give an explicit account of the range of conditions for which the model has been validated, and where the scope of the assessment necessitates use outside of this range, specific mention should be made of this fact, and some assessment should be given of the degree to which extrapolation has been taken. The data set used for validation should be independent of any data set incorporated in the model. Validation should be carried out against experimentally determined values, preferably measured in the environment to which the model is being applied. It is strongly recommended that a model that has not undergone such a validation process should only be used if there is no alternative, for example if it were the only model of its kind at an early stage in the development of modelling capability in a particular field. In such cases attention should be drawn to the speculative nature of the procedure.

It should be emphasised that comparison of the output of one model with the output of another model does not necessarily constitute validation; such a procedure constitutes a comparison only, although it may have merit as part of a validation procedure if the primary model has been well validated. This kind of comparison should be approached with considerable caution, and should be carefully justified for the cases considered. Scientific assessment involves examination of the validity of the description of the mechanisms that are modelled. This is of particular significance where it is necessary to investigate conditions that are outside the range within which the models have been validated. Application outside of the validated range will depend for its validity on the judgment made as to the robustness of these scientific descriptions in those circumstances. In such cases there should be an explicit statement of the conditions in which the model is judged to be applicable, and those in which it is not applicable. Responsibility in this matter falls on both model developers to provide the source of guidance, and on users to demonstrate that they properly appreciate the issues..

RMetS 1995 guidance.

8.1 Overview

Providing assurance of the quality of a modelling study can be achieved through three distinct procedures:

a Verification
b Validation
c Scientific assessment.

It is important that the user should consider the whole modelling assessment in demonstrating quality assurance and not limit the exercise to the dispersion model alone. For example, the model assessment is likely to include ambient monitoring data, emissions data and meteorological data, all of which are expected to include some degree of processing in addition to the dispersion model itself.

8.2 Verification

A computer model can be considered verified if a detailed examination has shown that it is a true version of the mathematical model which it incorporates, and that the coding faithfully reproduces the mathematical model approximations included in the algorithms. Ideally, the verification should be undertaken by someone independent of the computer programmer(s).

In circumstances where a proprietary model is being used the user should seek a statement from the supplier that the model (including version and release date) has been verified. It should be expected that established model suppliers would provide such certification as a matter of course.

8.3 Validation

A computer model can be validated with reference to an independent dataset, such as field data from a controlled release experiment or from ambient air quality measurements.

A controlled release experiment often yields a significant dataset (thousands of data pairs) allowing the user to undertake a formal validation exercise, such as the Model Validation Toolkit widely distributed by Olesen (1997, 1999, 2001) and the emerging American Society for Testing and Materials (ASTM) Standard Practice (Irwin 1999, or see http://www.harmo.org/astm/default.asp). Unfortunately these datasets do not always apply directly to the circumstances being assessed. This is important as a model can only be considered valid for a specific application if the circumstances being modelled are comparable with the circumstances of the field dataset. Inevitably, a model is often only validated for a range covering the majority, but not all, of the circumstances it may be applied to in practice.

In circumstances where a proprietary model is being used the user should seek references from the supplier that the model has been validated with controlled release experiments. The user should then determine whether the circumstances being modelled are comparable and hence, whether the model is validated for the intended use.

There are circumstances where local ambient air quality monitoring data may be available to provide a site specific model validation. This is considered critical if the circumstances being modelled are not comparable with field datasets from controlled release experiments. Typically, site specific datasets are limited, precluding the use of the recognised formal validation exercises. However, they can be useful in providing some degree of validation, and identification of systematic error (bias) and random error (uncertainty).

In undertaking a model validation exercise it is important not to rely solely on just one statistic, such as the correlation coefficient. Inclusion of the following may be considered as best practice:

a tabulation of observed and predicted data, noting the quality of the measured data and the uncertainty on the measurements

b summary statistics of the number of data pairs, minimum, maximum, mean and standard deviation of observed and predicted data

c graphical presentation of data as scatter plots and regression analysis with 1:1 best fit line and factor of two boundaries

d reporting of the bias, fractional bias and normalised mean deviation as measures of systematic error (bias)

e reporting of the index of agreement, normalised mean square error, Pearson's correlation coefficient, fraction of data within a factor of two and Root Mean Square Difference in Concentrations as measures of random error (uncertainty).

Some degree of pragmatism is required with emphasis placed on identifying the limits to which the model can be clearly demonstrated as validated for the circumstances in which it is being applied.

8.4 Comparing with other models

A further option is to compare the model with the results of another model; this can also include comparing the results from a numerical computational model with those from a physical model such as a wind tunnel. This is not strictly model validation although it can provide a useful check.

For the majority of industrial air quality modelling studies there is scope to utilise more than one proprietary model. The majority of the input data are similar and in the same format, and the model run times are in the order of hours. Although this adds to the time and effort required, and hence cost, there are a number of advantages:

a Under many circumstances, the models generate similar results. This can assist in demonstrating the robustness of the assessment.

b In circumstances where the models do not generate similar results there is the opportunity to investigate why. If this is done, then care should be taken to ensure that both models are appropriate for the situation being considered. In this case, the difference could give an indication of model uncertainty. This could be particularly useful when considering complex topography, building wake effects and atmospheric chemistry. However, even in a situation where uncertainty is considerable, the models may use the same approach, and so the difference would not then correctly indicate the level of uncertainty in the application.

Experience suggests that this dual modelling approach offers the opportunity for user training, enhancing an understanding of the limitations of models and their application.

A related approach is using two modellers to run each model; this provides opportunity for cross checking data input and model set up.

8.5 Scientific assessment

The scientific assessment of a model requires examination and understanding of the validity of the algorithms in describing the mechanisms being modelled. This is particularly important in considering the limits to model validation when referring to field data and in applications where the conditions in controlled release experiments are not strictly comparable to those of the assessment.

8.6 Validation of supporting data

Dispersion models usually require supporting data in the form of ambient monitoring data, emissions data and meteorological data.

Defra has issued guidance and provides training on the formal procedures for verification and validation of ambient air quality monitoring data.

Emissions data may be derived either by direct measurement, physico-chemical modelling or from information on the process type (source) activity and relevant emission factors. Defra has issued guidance and provides training on the formal procedures for verification and validation of direct measurements from stacks and commissions its own research on emissions from other sources such as road vehicles. Physico-chemical models require the same degree of verification, validation and scientific assessment described above. Defra has also issued guidance on the use of emission factors and activity data, and maintains an emissions factor databank. Note that derivation of activity data may require some understanding of the operating scenarios being assessed and the subsequent implications on emission characteristics.

9 AUDITABILITY

To ensure that there is a clear and transparent account of the exercise for inspection by interested parties.

BOX 11 –AUDITABILITY

An essential requirement in the documentation of a dispersion modelling exercise is that of auditability. The test in this respect is that the documentation should give a complete and transparent account of what has been done. Interested parties should be able to rely on the documentation in this respect, so that they can scrutinise, check, and if desired repeat what has been done without having to seek any further information. The audit procedure often proves to be the means whereby problems are first revealed. Auditability is enhanced by successful communication, and it is recommended that good use should be made of graphical and diagrammatic summaries, such as flow charts representing the adopted calculation strategy.

RMetS 1995 guidance.

9.1 Introduction

The true test of an auditable exercise is one that has been sufficiently documented to be repeated independently by a third party. This can be achieved by a line by line account of the modelling exercise, by use of checklists, or by a combination of the two. It is important that the model user should document the complete modelling process – from defining scenarios, calculation of emissions, selection of meteorological data through to post processing and interpretation – and not just how the dispersion model itself was set up and run.

9.2 The audit trail

Before embarking on a modelling exercise the user is advised to plan out each step, identifying the decisions that need to be made. Note that this requires the user to justify each decision. Moreover, this can provide a useful learning tool for model users.

9.3 Presentation in reports

For most audiences, a report on a modelling exercise needs to be concise, focussing on describing the circumstances being modelled and interpretation of the results. The use of technical appendices is recommended for including a detailed description of how each decision was made at each step of the modelling exercise (the audit trail). How these appendices are structured is for the user to determine, but the objective will be to provide all pertinent information that will enable an independent third party to repeat the modelling exercise and generate the same results.

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