ADMLC-R12

Guidelines for the Preparation of Short Range Dispersion Modelling Assessments for Compliance with Regulatory Requirements – An Update to the ADMLC 2004 Guidance

Endorsed by the Royal Meteorological Society

FOREWORD: 25 years of Atmospheric Dispersion Modelling Guidelines

The idea of developing guidelines on the selection and use of atmospheric dispersion models was first proposed in 1994 by Professor Richard Griffiths of the University of Manchester Institute of Science and Technology. The proposal was made in the context of comments in the environmental press, regarding the variable standard of environmental impact assessments that were being prepared for permit applications under the then new Integrated Pollution Control regime. The regime applied to industrial sites, rather than to other sources of air pollution, and many sites emitted pollutants whose dispersion had to be modelled for permit applications. Professor Griffiths proposed that some guidelines should be prepared that could inform and promote good practice in atmospheric dispersion modelling, and that would support the reputation of the emerging profession of air-quality specialists.

In 1994 the Royal Meteorological Society (RMS) had recently established the qualification of "Chartered Meteorologist". This made RMS the first professional body with a chartership explicitly for atmospheric specialists - including for air-quality specialists (other air-quality bodies had not yet been formed). Professor Griffiths therefore proposed to the RMS that they set up a technical group of specialists in air-pollution meteorology and air-dispersion modelling, in order to develop and publish some dispersion modelling guidelines. RMS welcomed the proposal, and Professor Griffiths agreed to chair the group - whose members came from a range of professional bodies and backgrounds e.g. regulators, research institutes and consultancies. This diversity of bodies and backgrounds has been a continuing and valuable feature of how the guidelines have been developed and updated over 25 years. The first guidelines were published by the RMS 1995, and outlined general principles and practices for effective dispersion modelling.

The late 1990s and early 2000s were a time of rapid expansion in air-quality regulation and professional practice. For example they saw: the advent of Local Air Quality Management in 1997; the start of the Dispersion Model Users' Group (DMUG) as a practitioner forum; and the formation of the Institute of Air Quality Management (IAQM) in 2002. This expansion meant that dispersion modelling was not only needed for industrial sites, but increasingly for other types of source e.g. aviation, intensive agriculture, and especially for road traffic. There were also important developments in dispersion modelling methods e.g. faster computers, more detailed input data on emissions and meteorology, and new air-quality standards for comparison with model predictions. By the early 2000s it was clear that the original 1995 guidelines needed updating in order to cover these developments.

In 2003, members of the RMS and other relevant bodies had initial discussions on how to arrange an update of the guidelines. The bodies included the newly-formed IAQM, and also the UK Atmospheric Dispersion Modelling Liaison Committee (ADMLC). ADMLC had been formed in 1978 as a group of scientists working mostly for government in dispersion research and prediction, in order to review dispersion topics and to produce technical summary reports (starting with the R91 report in 1979). ADMLC was therefore an established group of specialists that was similar to the original group set up for the 1995 guidelines; moreover, some ADMLC members had links to IAQM and DMUG. It was agreed that ADMLC would "host" the work of updating the guidelines – which was done in consultation with the other bodies. The updated guidelines were published in 2004, as a revision to the 1995 RMS Guidelines.

In the years since 2004, the science and the profession of air quality modelling and assessment have continued to develop rapidly e.g. the IAQM attained a membership of over 500 in 2019. This has meant that a further update of the guidelines has been needed, and the work has again been "hosted" by the ADMLC in consultation with the RMS, IAQM and others. The latest 2021 guidelines are the result of that work.

The importance of air quality and atmospheric dispersion science is set to continue over the next 25 years, and so will the need for science-based guidelines that outline and promote good practice in dispersion modelling. Arrangements for preparing the guidelines may evolve, but the pattern of consultations between different bodies is well-established and should continue. In this way the guidelines will continue to reflect up-to-date dispersion science and practice, and to serve the needs of air-quality professionals and the environment.

Roger Timmis

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EXECUTIVE SUMMARY

The intention of this report is to guide professional air quality workers in the production of robust assessments by the careful consideration of the context, and the selection and justification of appropriate models and input data. It also advises on general methods of communicating the results of the assessment and considerations of variability, sensitivity and uncertainty. Recommendations are made for the recording of results and decisions in the form of an audit trail to aid subsequent inspection of the assessment process by third parties. Some specific areas where assessments are frequently found to be weak are addressed in a series of appendices.

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1 INTRODUCTION

In 1995 the Royal Meteorological Society 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).

This guidance was updated in 2004 by ADMLC (ADMLC, 2004) as agreed with RMetS and now the current document has been produced to take account of modelling and regulatory changes over the intervening years.

This guidance primarily relates to air quality assessments undertaken for the purposes of an environmental impact assessment, for example as part of a planning application or, for the purposes of securing a permit in accordance with environmental permitting regulations, or for local air quality management purposes. It should be noted that the precise requirements of assessments for planning and permitting may differ and care should be taken to ensure that both are catered for (e.g. Environment Agency, 2016; Defra, 2016; Scottish Executive, 2006; IAQM, 2018).

The overall process of assessing an air-quality situation with a dispersion model involves several stages and types of information. At its core, the process involves undertaking a source-pathway-receptor (SPR) calculation in order to predict how air pollutants may be emitted and transported, and how they may impact on sensitive receptors. A typical SPR calculation has 3 stages:

- Source estimation - when emissions are estimated;
- Pathway prediction - when dispersion is modelled; and
- Receptor evaluation - when predicted impacts are considered.

SPR calculations are usually preceded by a scenario-setting stage, when the pattern of source activity is defined. Also, they are usually followed by a compliance determination stage, when the impacts predicted at receptors are combined with other information (e.g. background concentrations) and compared with ambient air-quality standards.

The use of dispersion modelling to predict air pollutant pathways is an integral part of SPR calculations, and so of the overall assessment process. These guidelines focus mainly on the use of models for the central "pathway prediction" stage. Other stages of the overall assessment process are referred to in order to show how they link to the modelling stage, but the guidelines do not cover them in as much detail.

The document has been written principally for applications relating to controlled (as opposed to fugitive) releases. It provides specific advice on:

- determining the aims and scope of the assessment;
- software selection;
- data selection;
- addressing variability, sensitivity and uncertainty;
- comparison with relevant assessment criteria; and
- communicating results.

An updated list of references for guidance, regulations and relevant literature is appended, as are several short appendices which provide advice on areas which are frequently found to be weak in impact assessments.

It is worth stating at the outset that if a regulator is to be involved it is both efficient and good practice to secure prior agreement on the scope, method and objectives of the air quality assessment. Defining these requires a clear understanding of the purpose of the assessment and the expected audience.

2 AUDITABILITY

Air quality assessments have to be auditable so that another party may independently trace, and check the assessment through to its conclusions. This may be required for instance to justify the decision-making process or for regulatory checks.

Before embarking on a modelling exercise the user is advised to describe the problem to be addressed and how modelling will be used to help find a solution. There are potentially many aspects to this. One particular aspect would be to consider the level of precision required. For example, if the decisions to be made based on the assessment results are safety critical then it is important to have a high degree of confidence in the model predictions (e.g. Gant and Tucker, 2018). This means that the uncertainties inherent in the modelling process are well understood and within acceptable levels to ensure safety.

Once the problem to be addressed has been clearly framed, it is good practice to plan out each step, identifying and justifying the decisions that need to be made and showing that they are appropriate for the task in hand. This will make the creation of an auditable assessment more straightforward.

The origins of all input data, assumptions and information should be clearly stated and referenced:

- defined scenarios;
- source terms;
- relevant building locations and dimensions;
- topography, surface roughness lengths and other surface parameters;
- selection of meteorological data;
- justification of dispersion modelling method and software;
- choice and justification of averaging times;
- choice of receptors;
- acceptance criteria (relating to levels of harm or termination of a process)
- pollutant background levels;
- use of chemistry modules;
- deposition assumptions;
- other special model formulations.

The subsequent manipulation and analysis of modelling results should also be clearly laid out so that the methods used may be repeated independently. The analysis should include:

- determination of impacts;
- considerations of uncertainty;
- interpretation of results.

For most audiences, a report on a modelling exercise needs to be concise, focussing on describing the circumstances being modelled, the methods used 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 understand the selection of model parameters and variables and to test the validity of the results. Model files and some input data will be submitted in electronic format. These should be clearly labelled and referenced in accompanying documentation. The software version should be stated.

The assessment should be transparent, coherent and logical. The inclusion of model lists and run logs (in appendices) can be useful (however it is recognised that model log files do not always provide comprehensive model setup information). The creation of the assessment as a series of auditable steps should be viewed as an aid to the person who is undertaking the initial task as much as to any later customer or regulator. It often proves to be the means whereby assessment problems are first revealed.

Auditability is enhanced by successful communication, and it is recommended that, where appropriate, use should be made of graphical and diagrammatic summaries such as flow charts, representing the adopted calculation strategy.

3 MODELLING

There are many aspects to dispersion modelling that should be taken into account when commencing a study. In this chapter we discuss the most important of these: screening, detailed modelling, model selection, input data and systematic modelling.

3.1 Screening

A screening process should generally be undertaken prior to carrying out modelling (Defra, 2016; Environment Agency, 2010, 2016; DMRB, 2007; SCAIL, n.d.). This may save time and money for all concerned. The screening should use reasonably conservative assumptions so that environmental impacts are, if anything, overestimated. If the screening process predicts that the impact will be safely below statutory levels it is likely that no further assessment is required.

If screening shows that the impacts are above statutory limits, or the process contribution is above a certain percentage of a statutory limit (e.g. Environment Agency, 2016), then detailed modelling may be necessary.

If the proposed project is of national significance it is probable that a screening procedure will not suffice and detailed modelling will be required (see Nationally Significant Infrastructure Projects, NSIPs, Planning Inspectorate, n.d.; Scottish Government, 2014; Welsh Government, 2016).

3.2 Detailed Modelling

Where it has been determined that detailed dispersion modelling is required, the choice of which software to adopt for a particular assessment is dependent primarily upon the following:

- Is the software based on sound scientific principles?
- Has the model been validated against relevant experimental data?
- Can the software adequately describe the circumstances being assessed (see 4.4)?
- Is the output sufficient for the assessment?

Resource or time constraints should not be a key determinant in the choice of model, indeed careful planning of the assessment is necessary to avoid such issues. The procedure adopted should be related to the predicted or perceived risk and potential impact (environmental but possibly also business or reputational). A high risk/impact scenario may require a more involved investigation.

The modelling procedure needs to encompass both the source of atmospheric pollutants and all relevant influences upon dispersion through the atmosphere to the relevant receptors (human and ecological).

Contacting a regulator to agree a proposed method in advance of carrying out the detailed modelling may save time and effort for both parties.

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

3.2.1 Model selection

The chosen software should be suitable for modelling the scenario in question and producing the required outputs. Software developers should provide a manual with a discussion of the scope for which the software is applicable and has been validated (section 4.4).

The most commonly used dispersion models, at least for regulatory purposes in the UK, are based on an assumption of Gaussian type plume behaviour and typically have a range of applicability of some tens of kilometres when applied for statistical analysis and within constraints related to the meteorology, terrain and other local conditions.

Gaussian plume models are generally most accurate for situations with elevated point sources in open country, and where there are no significant building, terrain or complex meteorological effects on dispersion (De Vischer, 2014, cpt 2). Nevertheless, Gaussian models do have options to take some account of these factors and are frequently used for scenarios where they are present, although it should be understood that uncertainties will be higher.

Care should be taken with modelling for low wind speed (typically < 1 m s^{-1}) or calm periods, especially for low level sources (De Vischer, 2014, cpt 6). Low wind speeds can contribute to poor dispersion.

There may be circumstances where other types of model are more appropriate – for instance where the dispersion conditions are complex, such as around buildings, complex terrain or over longer distances. Such models may be Lagrangian or Eulerian in basis, use computational fluid dynamics (CFD) for the explicit calculation of air movement and dispersion around structures or terrain, or integral models that are able to model complex near-field effects and can transition to passive dispersion further downwind as the gas becomes more dilute (Blocken, 2015; Casey and Wintergerste, 2000; De Visscher, 2014; Environment Protection Agency, 2010; US EPA, 2017; Witlox et al., 2018). Wind tunnel data may also be extrapolated to the scenario in question (Robins, 2003). Recent work has compared Gaussian model and CFD predictions and wind tunnel results for very short range dispersion (<100 m) (Woodward et al., 2021).

3.2.2 Input Data for detailed modelling

The selection of appropriate input data to the modelling software is of the greatest importance for achieving representative outputs. The following are the most frequently used categories:

1. Source
2. Topography and surface parameters
3. Buildings

4. Meteorology
5. Modelling grid
6. Receptors
7. Deposition
8. Background concentrations
9. Atmospheric chemistry

3.2.2.1 Source data

Source data will include: pollutant types and characteristics that affect the dispersion (such as particle size and chemical form), emission rates, start time and duration, gas exit velocity and temperature, geometry (point, line, area), dimensions, height and location of the emission point(s).

Emission conditions may change with time or with meteorological conditions and such variation may need to be represented in the modelling. For example:

- where emissions vary with changing meteorology (e.g. surface particulate matter); or
- there are diurnally or batch process operating profiles; or
- due to variations in the process load; or
- where there is a lag time for secondary abatement to be effective at controlling emissions.

Emission rates (e.g. in units of mass of pollutant, or odour or radioactivity emitted per second) may be derived from manufacturers' specifications, monitoring data, combustion calculations, national fleet emissions and activity data, Best Available Technology Associated Emission Levels or Emission Limit Values (BAT AELs/ ELVs) (European Commission, 2018) or other guidance (e.g. US EPA AP42).

Source data should be referenced.

The calculation of normalised or reference flow conditions is a frequent source of error. In appendix A1 there is guidance on the derivation and use of normalised volume flow rates from ELVs to estimate pollutant emission rates. The calculation of emission rates from ELVs should be clearly laid out with comprehensive statements of both reference and measurement conditions.

In addition to point sources, emissions may take the form or approximate form of lines, areas, volumes or jets (e.g. Stocker et al, 2016). For instance, a row of unforced ventilation slits on a building used to house intensively farmed livestock may be considered as a line source with an emission rate of g m^{-1} s^{-1} or, in some circumstances as a volume source with an emission rate in g m^{-3} s^{-1}. Particulate emissions from a dusty site may be best represented as area emissions with an emission rate of g m^{-2} s^{-1}; the emission rate here may have a wind speed dependency (US EPA AP42). If the release has non-negligible initial momentum or buoyancy, plume rise may be important and it is necessary to use a source type that takes this into account. Details of source properties, geometries and data input requirements are typically found in the software's user guide.

Uncertainties in emission rates will exist for many scenarios, e.g. where monitored data has been used, and should be quoted where possible. It should be recognised that these will affect the overall uncertainty associated with the assessment. This is particularly important for short term assessments. In some cases, it may be advisable to perform additional modelling to evaluate the sensitivity of the solution to these uncertainties.

3.2.2.2 Topographical and surface land use data

In some instances, topographic data should be treated by the model. For example, some software may recommend this when slopes of greater than 10% are present within the modelled area. Topographic data may be supplied from on-line sources to an agreed format and density, reprocessed to some different density (to a format compatible with the software), or derived from raw data. The resolution should be sufficient to ensure that surface features that could affect pollutant dispersion are adequately represented. Advice on this may be found in software developers' guidance. The data source should be referenced.

Topographic data may also include surface boundaries e.g. between land and water at the coast or lakesides, or between cities and surrounding countryside. Model users should consider the possibility that local flows in such topographies may not be well represented by non-local meteorological data. Buoyancy-induced valley winds (katabatic and anabatic flows) and land sea breezes are further examples where non-local meteorological data may provide a poor representation, especially in stable conditions. The use of high spatial resolution prognostic meteorological data (1.5 km) may be beneficial in some circumstances.

Of the common surface use parameters, surface roughness or roughness length (usually in metres) is frequently the most important. It represents the mean height across an area at which the wind velocity tends to zero. It is sometimes referred to in the context of land use (e.g. city, town, rural, woodland, etc.). The software guidance notes should advise on the best way to estimate representative surface roughness lengths.

Surface parameters may vary with direction and distance from a dispersion site. Under some circumstances it may be important to ensure that these are represented. Failing this, it may be useful to model dispersion a number of times, varying the surface parameters, for instance where there are multiple significant wind directions and the parameter values vary across these directions. Modelling predictions may be very sensitive to surface roughness values, particularly for low emission heights.

Other parameters include the Bowen ratio or Priestley-Taylor parameter (which partition the surface heat flux into sensible and latent components), albedo (the fraction of incoming sunlight reflected back) and the minimum Monin-Obukhov length (a measure of the height at which buoyancy-induced turbulence is approximately equal to that induced by wind shear; at greater heights buoyancy tends to dominate). Note that over large urban areas the Monin-Obukhov length may be unable to fall below a certain value because of the significant levels of retained heat and building induced turbulence. Depending on the model used, a selection of these parameters may be considered and should be informed by a study of the local topography.

As with other input parameters, model sensitivity to the choice of values used for surface parameters should be understood, particularly if those values are the defaults for the software.

3.2.2.3 Building data

Buildings in the vicinity of a source may interfere with the dispersion and cause local enhancement of ground level concentrations through downwash and wake effects. Modelling predictions may be extremely sensitive to these effects and the uncertainties can increase markedly.

For industrial sources the US EPA (1985) recommends that downwash should be taken into account when there are local buildings with:

- heights greater than 40% of that of the stack, and
- within a distance of 5L from the stack

where L is the lesser of the building height and maximum crosswind width. However, these criteria may vary somewhat with different software packages.

The software guidance notes should provide details of when and how to include building dimensions and locations in the model. Note that some models are unable to account for building downwash effects on emissions from area or volume sources. Guidance from the software developers should be sought in these cases.

For road traffic assessments, individual building dimensions generally are not critical although due consideration should be given to local surface parameters, including roughness length, road width and street canyon dimensions (e.g. see Defra, 2016). This may not apply, however, at road intersections or near very large buildings, especially high-rise buildings.

3.2.2.4 Meteorological data

The selected meteorological data should be representative of conditions at the dispersion site.

Typically, meteorological data are derived from internationally accepted weather observation techniques (World Meteorological Organisation, 2018; UK Met Office, n.d.) at specified sites, or, from modelled or forecast data such as Numerical Weather Predictions (NWP).

For observed data it should be emphasised that geographic proximity alone is not a sufficient criterion for representativeness, and differences in both land use and terrain between the sites may well make the selection invalid. Examples of such differences would be between rural and urban, or inland and coastal landscapes.

If data are obtained from NWP, then the resolution and any pre-processing should be described. The US EPA (2017) recommends that representative measured data be used as a first choice, although the three-dimensional content of predicted data may, in some circumstances, make it superior to measured which is usually obtained at a single height.

If the dispersion model does not include specific terrain effects, the resolution of predicted meteorological data should be sufficiently fine to account for these.

In most circumstances it will be advisable to use up-to-date meteorological data. For instance, the westerly upland areas in UK are now experiencing heavier rainfall than in the past and summers may be drier. These factors may influence both pollutant dispersion and deposition. Changes in urbanisation around meteorological stations may also affect the degree of representativeness of older data.

These points should be borne in mind when justifying the use of meteorological data.

Occasionally the use of 'single line' meteorological data may be appropriate where the dispersion under particular conditions is being investigated.

In general, multiple years of meteorological data should be used to ensure that year to year variations are taken into account. The UK national environmental regulatory bodies advise the use of five years of consecutive meteorological data for environmental impact assessments with the results reported on the basis of annual statistics, not 5 yearly (e.g. Environment Agency, 2014). In other circumstances and for low risk cases it may be acceptable to use data representing fewer years.

High short-term local predictions may well occur at times of low wind speeds. Gaussian models tend to have a wind speed modelling threshold and will ignore periods when the wind speed is below this. Hence short-term periods of local high pollutant concentrations may be overlooked and it is advisable to check modelling run logs for the presence of significant numbers of ignored calm periods which could affect the model predictions.

3.2.2.5 Modelling grid

A modelling area encompassing the dispersion site and all relevant receptors should be defined. Such an area will comprise a grid of points at a specified distance apart. This resolution should be sufficient to enable capture of all appropriate maxima for both long- and short-term environmental standards. The spatial resolution required is likely to become less stringent as the plume is advected from the source and disperses. In some cases, separate model runs will have to be carried out with fine and coarse grids to ensure that no 'hot spots' have been missed close to the source and also to achieve coverage of the desired area. The dimensions and resolutions of these grids should be determined on a case by case basis but will be dependent on many factors including the source height, emission momentum and buoyancy, local meteorology, local buildings and terrain, receptor and source locations and the relevant environmental quality standards.

Short-range regulatory dispersion software usually offers the options of modelling on Cartesian or polar grids. There are advantages and disadvantages with each. With Cartesian grids, the grids are a uniform size but modelling times may be excessively long over a large area with a fine grid resolution. With polar grids, the grid resolution reduces with distance from the source or origin – care should be taken that there are sufficient grid points to capture the magnitude and location of the worst affected locations.

The location of regions where changes in plume development are rapid can be identified by examination of the modelled plume on a grid. Particular care should be taken with results from such regions as they may be especially sensitive to some model input parameters (see section 4.2).

3.2.2.6 Receptors

Receptor locations and types (human or ecological) should be identified from appropriate geographical information data and appropriately referenced. In some circumstances it will be appropriate to consult an ecologist (CIEEM n.d., IAQM, 2018). The relevant statutory or other exposure limits should be applied to each receptor (Defra, n.d.; Air Quality in Scotland, 2018; Air Quality in Wales, 2018). Defra has advised that these are to be considered only for locations where members of the public (not workplaces) may be exposed, e.g. annual means outside residential addresses or hourly percentiles where the human population might reasonably be expected to be exposed for timescales of the order of an hour (Defra, 2016).

Pollutant levels at locations of specific receptors may be determined in addition to a modelled grid but the results should always be checked against those of the grid. This may highlight anomalous results and will help to ensure that correct grid references have been used for the receptors.

3.2.2.7 Deposition

Deposition can occur under both wet and dry conditions. Pollutants are removed from the air in wet conditions by falling water droplets and other forms of precipitation. Under dry conditions, pollutant species are directly deposited onto surface features, typically vegetation.

Plume depletion (whereby one or more chemical and/or physical processes act to deplete the concentrations in air of a 'plume' as it is advected by the wind from the source of the release) will occur concurrently with deposition and can be accounted for in some software. Ignoring deposition and depletion will lead to more conservative predictions for plume ground level air concentrations.

Further guidance on modelling deposition is given in appendix A3.

3.2.2.8 Background data

Total concentration levels are a combination of contributions from the emissions under investigation, foreground emissions and the general background. For example, busy roads and major industry may be considered as foreground sources if receptors are sufficiently close that the pollutant concentrations at these are elevated above the background. These foreground levels may be estimated by dispersion modelling for the local sources.

Therefore, in order to determine the total environmental concentrations of pollutants it will be necessary to add background and foreground values at the individual receptor locations to the process contributions predicted by the modelling procedure. The data should be as representative as possible of the backgrounds at the receptors concerned. Where receptors are close to sources of pollutants (e.g. busy roads, major industry) it is likely that large scale average values such as 1 x 1 km squares (Defra, 2015) or 5 x 5 km squares (APIS, 2016) will be significantly lower than the concentrations at such receptors. Defra run Automatic Urban and Rural Network (AURN) and Local Authority monitoring networks (continuous monitors and diffusion tubes) may be good sources of more accurate localised data (Defra, 2015). This is especially likely to be true for nitrogen dioxide and particulate matter. In the vicinity of oil refineries sulphur dioxide levels are likely to be elevated and may show strong temporal and spatial fluctuations.

Background levels for many species are only measured at a few discrete locations around the UK. In using this data to arrive at a probable background value for the receptor in question, consideration should be given to the nature of the area surrounding the monitoring site, as well as its proximity to the receptor. For instance, elevated levels of certain metals or polycyclic aromatic hydrocarbons may be associated with industrial processes where coal or coal-based products are burnt.

Defra have produced guidance on the estimation of backgrounds for local air quality purposes (Defra, 2018). In the Environment Agency guidance for screening of short term impacts the annual average background levels are multiplied by two to obtain a value for the hourly background (Environment Agency, 2016). Where detailed modelling has been used, the Environment Agency requires either conservative or representative background data be used (Environment Agency, 2014). If continuous monitoring data is available statistical analysis may be used to consider the likelihood of a coincidence of high backgrounds and process contributions.

In general, background values when considered over long averaging times (e.g. 1 year) will be more reliable than over short term periods when large fluctuations may occur.

3.2.2.9 Atmospheric chemistry

An understanding of the fundamental physical and chemical processes and assumptions on which atmospheric chemistry modelling is based is essential for deriving robust predictions.

If NO oxidation (via reaction with O_3) is to be predicted it is important to state and reference the expected proportion of NO_2 in the source emission. Note that fractions of NO_2 in NOx from gas engines may be much higher than from other combustion processes. O_3 levels should be justified and referenced. In general, data should be obtained from a continuous monitor with hourly averaged data. Evidence from more than one monitoring site may strengthen the case for a particular value or dataset.

The Environment Agency has provided guidance on the proportions of NO_2 within NO_x (Environment Agency, 2012a). The guidance applies to NO_x with a primary NO_2 content of ≤10% and stated that reasonable worst-case oxidation assumptions include 70% of long term NO_x as NO_2 and 35% of short term NO_x as NO_2.

Note that where traffic emissions are under consideration, local monitoring data for NO_2 and NO_x, when available, should be given precedence over modelled predictions.

3.3 Systematic modelling

It is rarely, if ever, sufficient to run a model for just one set of input parameters. Variability in the input data (e.g. emission rates, meteorological years) should be accounted for, sensitivity of the outputs to certain parameters should be investigated, the effects of approximations in modelling methods allowed for and the results of validation exercises discussed. In short, an estimate of the overall uncertainty in the results should be derived and presented. These topics are discussed in more detail in the next chapter. Here it should be noted that the systematic planning and result recording of multiple model runs in which these factors are investigated is of crucial importance in dispersion modelling. Such methodologies should be clearly laid out in the accompanying audit trail.

4 UNCERTAINTY

A typical dispersion model will require the user to input a number of variables in addition to meteorological data, which itself will include a range of parameters for each unit of time modelled. A prime objective of all modelling studies should be to demonstrate a high degree of robustness. This requires an understanding of the possible scope of *variability* in input parameters, the *sensitivity* of the model to input parameters which, in addition to an understanding of inherent limitations of modelling processes, may be used to address the inherent range of *uncertainty* in model outputs (e.g. Arya, 1999).

These terms will now be discussed in more detail, with reference to some of the parameters that are used in dispersion modelling.

Finally, the importance of understanding, assessing and presenting these terms is emphasized in the context of comparisons with measured data and public communication.

4.1 Variability

Variability refers to the inherent heterogeneity or diversity of data in an assessment. It cannot be reduced for many processes but should be understood and characterised. In dispersion modelling the observed meteorological data is an example of such variability. Another is spatial and temporal variation in source emission parameters; in fact probably most parameters in dispersion modelling will have a degree of variability.

In many circumstances it will be appropriate to investigate the reasonable worst-case situation in a given scenario. Hence the recommendation to use five years of representative, consecutive meteorological data with the selection of those predictions derived on the basis of the worst year for a given environmental quality standard (Environment Agency, 2014), together with emissions at the relevant ELVs.

Consideration of the variability of exhaust gas emission parameters in this respect should also be undertaken – for instance ground level concentrations may be enhanced at times of reduced upward-momentum or buoyancy of the plume, as well as at times of increased emission rate. This is of particular relevance for short term percentile-based standards.

4.2 Sensitivity

A high *sensitivity* to model input parameters is demonstrated if a relatively large change in the magnitude or significance of a prediction is caused by a small change in an input parameter. Examples of this are:

- the onset of plume downwash when the plume is entrained in the turbulent wake region of a building may be sensitive to the building dimensions;
- when the effective stack height (a function of stack height, diameter, exhaust velocity and temperature) is close to predicted boundary layer heights;

- when a prediction is close to a threshold value for an environmental assessment level or environmental quality standard;
- when setting up a model for dispersion from road traffic emissions, the ground level concentration at nearby receptors will be sensitive to the number, location, length and traffic density/make-up of the roads;
- the influence of surface roughness length (or other surface parameters) on predicted ground level air concentrations from low emission heights;
- under very stable or unstable conditions with wind speeds ≤ 1 m s^{-1}.

Sensitivity checks, used in conjunction with validation studies (see section 4.4), can give confidence that predictions are below certain values or help understand model uncertainties.

When discussing significant sensitivities, it is necessary to make reference to quantitative changes in both the selected input parameter and modelled result. The importance of the changes should be described, particularly when a predicted value is close to an environmental standard.

Many input parameters to dispersion models are approximations and their magnitudes may be, to greater or lesser extents, debatable. In this regard it may be useful to determine the effects on model outputs across ranges of these input parameter values where high output sensitivities might reasonably be expected. It may be appropriate to display the results in the form of a table or matrix.

Unsubstantiated assertions as to the insensitivity of the results to certain factors should be avoided. Arguments will be more rigorously made when carried out with reference to quantitative examples.

Global sensitivity analysis, where input parameters are varied simultaneously across the parameter space, can provide useful information on model behaviour. For example, it can highlight interactions between model inputs that may be missed in local (or one-at-a-time) sensitivity analysis (Gant et al, 2013).

4.3 Uncertainty

There are many causes of uncertainty in dispersion modelling, for example:

- temporal and spatial variability in emission and atmospheric parameters;
- the equations and algorithms used in the model (both in the derivation of secondary meteorological parameters and of predicted concentrations) that are only partially representative of the physical situations being modelled;
- the non-deterministic nature of the turbulence and diffusion processes.

Hence different models using differing approaches and simplifications should not be expected to give identical results from identical input data. In principle, the magnitude of uncertainty in an assessment can be reduced with the use of more detailed and higher accuracy data and with more realistic modelling procedures. An understanding of the range of software performances for differing types of modelling scenario will assist here (see section 4.4.1).

The level of uncertainty is likely to be high in scenarios where the model output sensitivity is high (see section 4.2). For instance, in the wake regions behind stacks and buildings the model sensitivity can be high and the levels of uncertainty are also increased.

Another example lies in meteorological data that will rarely be specific to a particular location. Even if it is, it cannot give precise predictions of future dispersion conditions or even of conditions at differing heights and horizontal locations from that of the measurement position. Hence there will be an intrinsic uncertainty in dispersion predictions arising from the necessary use of meteorological data. If more than one model or meteorological data pre-processor can be run for a given scenario, the results will provide some indication of the uncertainty arising from the model selection. Examination of data from more than one meteorological site in the region of the dispersion site for a particular year may help to identify particular parameters which contribute to uncertainty.

The required accuracy of a prediction may depend on the relative magnitude of the relevant air quality standard and also the size of the background. If the prediction is low in comparison to either of these the accuracy may not be critical.

As mentioned earlier, in some circumstances use of data representing a reasonable worst-case scenario may be preferable, for instance where it is desirable to avoid breaches of environmental quality standards. This would involve using the most adverse (greatest) results (against a particular environmental standard) from five years of meteorological data and assuming continuous emission at ELVs (which, by definition, should not be exceeded). Note that the worst result may occur in different years for different environmental standards.

4.4 Fitness for Purpose – Model Evaluation (Validation)

Model evaluation is a means of ensuring a model's fitness-for-purpose. It also helps the user, or a decision maker, to have confidence in the model's predictions. A high-level outline of a structured approach to model evaluation that can be applied to any predictive model is described below.

The model evaluation process usually consists of a number of basic elements carried out in sequence or as a well-defined "protocol". Model evaluation protocols have been developed in the past for the purpose of assessing predictive models. The main elements of model evaluation are that:

- The underlying model should have a sound physical basis (Scientific assessment);
- The computer implementation of the model should be consistent with its mathematical basis (Verification); and
- The model should represent reality to an acceptable degree (Validation)
- The interaction between the user and the model should be considered (User-oriented assessment)
- The level of uncertainty when evaluating and using the model and its effect on output should be considered (Sensitivity and uncertainty analysis)

The rationale behind this structured approach is that each stage is dependent on the previous one having been carried out. There is little point in validating a model which has been programmed incorrectly and there is little point in programming a model which is not scientifically robust. That does not mean that such faults do not happen in practice; a model evaluation protocol should therefore be designed to help to detect them. Omitting any of the stages in a model evaluation is based on the assumption, or evidence, that the stage has been carried out previously, or there is appropriate justification for its omission. For example, if there are no relevant validation data, or the generation of new data is not practicable, then emphasis should be placed on other stages of the evaluation. This limitation should be acknowledged and highlighted when documenting the evaluation.

Before model evaluation can begin, it is necessary to establish the specific model, or models, to be evaluated. It is also necessary to establish the intended application area (purpose) of the model including which inputs and outputs will be used. This stage is important, because the comparative elements of the evaluation, such as validation and sensitivity and uncertainty analysis, depend on the scenarios to which the model will be applied. It also helps to ensure that the depth of evaluation is proportional to the level of use of the model. Other pre-evaluation tasks are to define who will use the model, how quickly the model will need to run, the required inputs/outputs of the evaluation and whether an existing protocol can be used to meet these requirements. The output of a model evaluation may be a single report describing all the stages, or may be a collection of individual reports, describing the outcome of each stage. In this case, an overarching master report may be necessary to provide an overview and to identify remaining gaps in the evaluation. The main requirement of reporting evaluation is to provide evidence that the stages have been carried out.

Pre-evaluation tasks need not be particularly onerous, and may simply involve defining the model, its purpose, who is to carry out the various parts of the evaluation, and what the outputs will be. At the end of the model evaluation, it is worthwhile undertaking a post-evaluation exercise in which the suitability of the protocol is reviewed and recommendations made.

Validation is a critical stage of the evaluation process. It is the stage that people most easily relate to and can be the most time consuming. The amount of emphasis to be placed on validation should be decided, in relation to that given to the other stages of the evaluation. It is also necessary to consider which datasets the model predictions will be compared to, how the model will be compared to the data and the level of agreement with the data to be expected from the model.

These tasks are not straightforward and require forethought and planning to ensure the relevant quantities are compared in a relevant way. Determining what constitutes a "good" or "acceptable" agreement with data is also difficult and often based on previous validation exercises of similar models.

An inherent property of model development is that it is an on-going process as models are refined and updated. The area of application of the model may also change as new uses and scenarios evolve. Model evaluation is part of the process of model improvement, rather than an isolated pass/fail test and the level of evaluation should be commensurate with the level of change in the model. The model evaluation process, when carried out fully, is time consuming and carries associated cost which can easily be justified in terms of increased confidence in predictions.

However, it may be relevant to apply a subset of the process when evaluating an updated model.

When an update refers to a new capability, or modelling physics, then a more rigorous evaluation may be needed, but not necessarily the full model evaluation process. In the pre-evaluation tasks, it is necessary to identify whether the evaluation is being applied in its entirety to a new or existing model, or whether it is being applied to an updated version of the model. In the latter case, evaluation can be seen as checking that predictive changes from a new, updated, version of the model relate only to the changes made, i.e. that particular updates or improvements have not impaired the function of the model in some other way, and that the update functions as planned.

Examples of model validation and evaluation can be found in: CERC, 2017a; Coldrick, 2017; US EPA, 2017; Harmo, 2017: Irwin, 2017.

4.4.1 Commercial models and field trials

Commercial software developers will reference relevant validation studies for their products, but it is unlikely that a model can be validated for all the scenarios it will be applied to in practice.

It is important to understand the limitations of the validation. Uncertainties in model predictions will be specified under various conditions and should be taken into account when presenting results. The modeller should state where modelled scenarios lie both inside and outside the range of these specified conditions. Care should be taken when using models for scenarios that are outside the range of validated conditions. Some degree of expert judgement is required to understand the implications for uncertainty estimation. An understanding of the physical basis of the model algorithms will aid in scoping the uncertainties.

Validation documentation should always be referenced and, if the modelling has been used for regulatory purposes, should be publicly available.

4.4.2 Other comparisons with measured data

There are circumstances where local ambient air quality monitoring data may be available to provide a more limited, site-specific model validation (Defra, 2016, paras 6.10 and 6.11). 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 (variability).

Toolkits for model evaluation have been developed and can be used to test against measured data (CERC, 2017b; HARMO, 2017).

4.4.3 Comparison with other modelling software

A further option is to compare the results from one model with those of another that is intended to model the same type of scenario under consideration. This is not model validation although it can provide a useful check. If both models incorporate "sound science" and have been validated for the type of application, then the range is indicative of the amount of uncertainty that exists in the "state of the science" for that particular case.

For the majority of industrial air quality modelling studies there is scope to utilise more than one model. For the most commonly used commercial models the majority of the input data are similar and in the same format, and the model run times are in the order of tens of minutes to hours. Although running multiple models adds to the time and effort required, and hence cost, there are a number of advantages:

- Under many circumstances, where models are appropriate for the situation being considered, the models generate similar results. This can assist, though not always, in demonstrating the robustness of the assessment and provide confidence in the results.

- 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.

Note that output similarities or differences may not correctly indicate the level of certainty or uncertainty in applications in all situations i.e. where models use the same approach.

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

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

Finally, the results from a dispersion model can be compared with those from a site-specific physical model in a wind tunnel experiment or results from high quality Computational Fluid Dynamics (CFD) simulations (see section 3.2.1 and references therein). The capabilities and limitations of these datasets should be considered carefully, e.g. scaling issues, wind meandering and uncertainties in atmospheric boundary-layer profiles with CFD.

4.4.4 Data referencing

In comparing modelled predictions with actual measurements it should be borne in mind that dispersion models work on the basis of averaged collections of data (ensemble means). Measured data will represent only a few of the possible manifestations of these and will inevitably differ to some extent.

Hence, as previously stated, the model user should address the issue of variability and give some estimate of the uncertainty that attaches to the modelling results. 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.

4.5 Presenting Uncertainty

Given the uncertainties in input data and model processes it will be difficult to present precise numerical limits to predicted pollutant concentrations. Nevertheless, by means of a consultation of relevant validation documents, boundaries of the uncertainties under well-defined conditions can be quoted. Given that the circumstances of the actual modelled scenario will vary to a greater or lesser degree from those of the validation, the uncertainties are also likely to differ. The use of conservative modelling assumptions, such as emission rates at ELVs and worst-case meteorological data, will not reduce this uncertainty but will shift the range of possible values to a more conservative position. A discussion of these considerations will help to put the predicted value into context.

4.6 Uncertainty and public communication

Failure to address the issues discussed here may result in a 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 assessment as a whole is discredited, and the potential usefulness of the information lost.

5 PREPARING AN AIR QUALITY ASSESSMENT REPORT

Whilst the actual sections of an air quality report may vary to some extent, in general the following would be expected.

5.1 Assessment Introduction

An opening section with:

- the purpose of the study;
- information on the background to the proposed installation;
- an outline of the development with the principal sources and pollutants;
- a description of the surrounding buildings, area and receptors, both human and ecological (much use can be made here of map, satellite and ground-based photography on the internet);
- consideration of the relevant environmental quality standards;
- the objectives and scope of the assessment; and
- based on the preceding, a reasoned explanation for the selection of software used in the assessment (for instance, the scope for modelling the effects of buildings and complex terrain in some software can be limited - demonstrate that the software chosen is appropriate).

5.2 Model Input Data

An extended section on modelling input data, possibly with many sub-sections, in which reasoned and referenced arguments are provided to support the selection of the data should include:

- description and data references of all relevant pollutant sources including all relevant flow and emission parameters;
- full details of calculations for the derivation of normalised flow rates (see appendix A1 for an example of how to calculate the normalised flow conditions and emission rate for a typical combustion scenario);
- details of abnormal short- and long-term emission conditions (see appendix A2);
- surrounding topography (see section 3.2.2.2);
- building data (see section 3.2.2.3);
- meteorological data (see section 3.2.2.4);
- land use parameters such as the Bowen ratio, albedo, minimum Monin-Obukhov length (see section 3.2.2.2);
- modelling grid resolution (see section 3.2.2.5);
- selection and location of receptors (see sections 3.2.2.5 and 3.2.2.6);
- selection and use of deposition parameters (see section 3.2.2.7 and appendices A3 and A5);
- background pollutant concentrations – Air Quality Management Areas (AQMAs), sources of data, evidence or considered arguments why the data is representative for each receptor, multiplication factors for background level depending on pollutant and statistical parameter (see section 3.2.2.8);
- atmospheric chemistry (see section 3.2.2.9);

- radiation dose and radioactivity; and
- choice of output parameters (including modelling time units, averaging times, statistical short term percentiles) with consideration of all relevant legislation and environmental quality standards for human and ecological receptors.

References to guidance documents for air quality standards and objectives for the UK and devolved administration are given in section 3.2.2.6. These list the relevant atmospheric pollutants and their long- and short-term statistical environmental quality standards. The Environment Agency’s guidance on detailed modelling also contains this data together with a more extensive list of substances and their environmental assessment levels (Environment Agency, 2016). Information on habitat critical loads may be found on the APIS website (APIS, 2016).

5.3 Running the Model

A description of all model runs undertaken, including the sensitivity analyses, should be included (see section 4.2). These can be summarised in a model run log.

5.4 Model Results and Their Communication

An air quality assessment can generate significant quantities of results and analysis. Include only those that are relevant to the study objectives and at the same time demonstrate the robustness of the assessment.

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

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

- Is there clear reference to and explanation for the selection of relevant assessment criteria, such as air quality environmental standards, odour requirements, etc.? Where multiple standards are involved, these may be most clearly shown in a table.

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

- Are process contributions and predicted environmental concentrations (process contribution plus background) clearly justified, presented and differentiated?

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

With regard to the presentation of data, the following should be borne in mind:

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 there. For instance, in permitting applications when presenting modelling predictions for pollutant levels, the table should include, besides the modelled process contributions, relevant air quality criteria, background air quality data and predicted environmental concentrations (i.e. process contributions plus background) for direct evaluation. Columns and rows should be clearly labelled and units included. Every table should have an accompanying title and explanatory text.

Graphs can assist in the interpretation and presentation of results. Axes and data should be clearly labelled and units included. As for tables, there should be both an accompanying title and explanatory text.

Contour plots are a common means of illustrating the scale and magnitude of an air quality impact. Plotting the contours onto a suitable base map assists in this, particularly when key features, such as sensitive receptors, terrain features and sources of air pollution are identified. Note that the interpolation method (kriging, etc.) should be specified as this can lead to differences in the final contour plots. Contour plots should include a scale and northing, and extend to show all relevant features. Colour–coded contours associated with concentrations or other parameters should be clearly labelled.

Each table, graph and contour plot should be given a unique identifier which is referred to in the text.

Discussions of uncertainty can then be provided on the basis of sensitivity analyses, the input data variability and the validation documents (see section 4). It is likely that the uncertainties quoted in the validation documents will give minimum values for the bulk of scenarios. This is because meteorological data will not be obtained at the site in question, emission data will be less well characterised and terrain and building effects will be different from the validation case.

5.5 Discussion and Conclusions

Discussion should be made with reference to the objectives of the assessment and modelling results. 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 an impact 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.

There should be an accounting for uncertainties within the final sections. The predictions should be considered within the context of these and may be seen as invalid until this is done.

Results should always be fully quoted as numerical values in any discussion of their significance. Avoid quoting numbers to more significant figures than are warranted by the input data or modelling method. A significance discussion should include the fraction of an environmental standard that is contributed by background, any foreground and the process contribution as well as the headroom available (i.e. the ‘space’ between the sum of the contributions and the standard).

The modelling inputs and meteorological conditions which lead to the worst impacts or exceedances of standards should be highlighted together with a consideration of their likelihood of occurrence.

A competent modelling study will identify the physical dispersion processes that accompany adverse impacts - for example, if an impact is due to high-wind-speed knock-down of a buoyant elevated plume, looping under unstable conditions or stable conditions involving low-level releases. This is partly for reasons of quality assurance (is the predicted adverse condition consistent with the source type?) and partly to inform mitigation of the adverse situation.

The results of sensitivity analysis should be extensively discussed if modelling shows that the predicted impact is high at one or more receptors.

All conclusions should be made explicit and expressed in a manner that bears a clear relationship to the stated objectives and to the results obtained from the modelling procedure.

5.6 Quality Assurance

There should be a section on quality assurance in which it is demonstrated that the work is fit for its specified purpose. The section should cover both the input data and the model itself.

The use of input data has already been discussed (see section 3.2.2). Here it is reiterated that the source of input data and associated uncertainties with quoted values should be stated. If accessed from the internet, the site and accession date should be given.

It is expected that the bulk of assessments will be carried out with commercial or proprietary software which has evidence of quality assurance for its application to a range of scenarios. The extent to which the software developer’s quality assurance may be applicable should be discussed in the report. Circumstances in which there may be greater uncertainty over the assurance coverage will require more discussion.

Appendices

A1 Normalised flows

The determination of gaseous emission rates from many processes is made with reference to emission limit values in the reference documents for best available techniques (BREFs) (European Commission, 2018) where they are quoted in terms of a mass of material emitted per normalised volume, e.g. mg/Nm^3. The normalised volume refers to a volume of dry gas at standard temperature and pressure, i.e. 273 K and 1013 hPa or 1 atmosphere, whereas the actual flow conditions are often at a higher temperature. Furthermore, the gas may contain water vapour and have a reduced oxygen content if combustion has been involved. The oxygen content is specifically stated in the BREF for those processes where it may have been altered. All these factors should be corrected for, so as to derive the normalised volume flow (b, Nm^3 s^{-1}) from the actual flow (a, Am^3 s^{-1}).

The general formula for the conversion is:

$$b = a.\left[\left(\frac{273}{T}\right)\cdot\left(\frac{P}{101.3}\right)\cdot\left(\frac{100-m}{100}\right)\cdot\left(\frac{20.9-l}{20.9-n}\right)\right]$$

where T and P are the temperature (K) and pressure of the actual flow (kPa), respectively, m is the moisture content percentage (by volume) of the actual flow, and l and n are the oxygen content percentages (by volume for dry gas, i.e. as measured with the water vapour removed) for the actual and specified conditions, respectively.

Note that a temperature in ^{0}C can be converted to K by adding 273 and that for most processes the pressure is unlikely to vary very much from atmospheric, hence the pressure correction can be usually ignored. The specified or reference oxygen percentage for a particular process can be found in the BREF or BAT conclusions documents, e.g. for kiln activities and the production of cement it is 10% oxygen by volume (European Commission, 2018).

Hence, for a gas flow in which the following parameters were measured:

- Temperature 400 ^{0}C (i.e. 673 K)
- Pressure 101.3 kPa
- Moisture content 5%
- Oxygen content (in dry gas) 8%
- Reference oxygen content for process 10%
- Actual flow 100 m^3 s^{-1} (calculated from the cross-sectional area of the stack or emission point, m^2, multiplied by the actual emission velocity, m s^{-1})

the normalised flow rate (b, Nm^3 s^{-1}) is given by

$$b = 100.\left[\left(\frac{273}{673}\right)\cdot\left(\frac{101.3}{101.3}\right)\cdot\left(\frac{100-5}{100}\right)\cdot\left(\frac{20.9-8}{20.9-10}\right)\right]$$

= 45.6 Nm^3 s^{-1}.

If the emission limit value for a particular pollutant for this process is z mg Nm^{-3} then the emission rate R (g s^{-1}) will be given by

$$R = \text{z.b. } 0.001$$

Hence for an emission limit value of 50 mg Nm^{-3} for the conditions just described, the emission rate would be

$$R = 50 \times 45.6 \times 10^{-3} \text{ g s}^{-1} = 2.3 \text{ g s}^{-1}$$

A2 Abnormal emissions

In the event of a failure of a pollutant remediation step (e.g. acid gas removal by injection of lime or heavy metal removal by injection of carbon dust) the process will emit at the full, pre-remediation pollutant concentration. This is known as abnormal emission.

In the Industrial Emissions Directive (IED) for waste incineration and co-incineration plants, abnormal emission rates are allowed for up to 4 hours at a time and for a maximum of 60 hours in a year (European Commission, 2014). If the remediation efficiency is high (e.g. ~ 99%) then abnormal emissions can significantly increase both the short term and long term emissions.

In order to estimate the abnormal emission rate the efficiency of the remediation step should be known. If this is q %, (i.e. the remediation removes q % of the pollutant in a gas stream) then the abnormal emission rate p (g s^{-1}) will be given by:

$$p = 100 \cdot \frac{R}{(100 - q)}$$

where R is the emission rate with the remediation functioning.

Hence if the remediation efficiency for a particular process is 90%, the abnormal emission rate will be calculated as:

$$p = 100 \cdot \frac{R}{(100 - 90)}$$

$$= 10 \cdot R$$

i.e. the abnormal emission rate will be ten times the remediated rate. However, it should be noted that for some circumstances the IED will set an abnormal ELV of less than 10 times the normal ELV.

Manufacturers should provide remediation efficiencies for their equipment. This data should be used to estimate abnormal emission rates and should be fully referenced.

A3 Deposition

Material from plumes will, in many cases, come to ground or be deposited onto surfaces near ground level. This can be explicitly modelled in some software.

For instance, in some ecological assessments, nitrogen and acid deposition to vegetation will have to be predicted. In human health risk assessments, the deposition to food sources of particulates containing certain heavy metals, dioxins, furans or dioxin-like polycyclic aromatics should be modelled. Deposition of large dust particles may be a source of nuisance around some types of site.

Deposition of air-born pollutants to ground level can occur through both wet and dry processes. Wet deposition occurs via one of two processes. Washout, where precipitation (in liquid and solid forms) sweeps through and removes pollutants from the air. And rainout, where water condenses on, or absorbes, pollutants from the air (in elevated cloud or fog/mist), which then falls to the ground. In this case, the mean plume height can be some distance from the ground. For example, the Environment Agency and National Resources Wales only require wet deposition of HCl and HNO_3 to be considered for short-range modelling (< 10 km) as the process is taken to be insignificant for other species.

With dry deposition, pollutants in the plume come into direct contact with vegetation, soil or the built environment and are transferred. The precise physical and chemical processes involved will vary with pollutant species and surface type. Deposition characteristics, often expressed as a deposition 'velocity' or surface 'resistance', can be defined for particular species and surface vegetation types (and often vary diurnally and seasonally). The pollutant flux to the surface is calculated from the product of the pollutant ground level concentration and the deposition velocity.

Guidance notes of the software used will give more details on the physical processes involved and the parameter selections that have to be made but these may include:

- Pollutant species;
- Particle size and density;
- Deposition surface (e.g. woodland, grassland, bare earth);
- Season;
- Time of day; and
- Meteorological conditions (e.g. wind speed, precipitation rate)

Some or all of these parameters may have to be taken into account and their use justified. Likewise, if some are to be ignored, the reasons for this may also have to be given.

Plume depletion occurs at the same time as deposition and some software will allow the user to take this into account.

Note that for ammonia the concentration dependency of the deposition velocity will have to be considered when assessing the impact of intensive farms (Environment Agency, 2010).

A4 Odour Modelling

The human response to odoriferous chemicals is complex – as well as concentration and species type, the time and location, the speed of onset and frequency of occurrence are also crucial factors (Environment Agency, 2002, 2007; IAQM, 2018). Odour concentrations may be specified in terms of odour units per m^3 and odour emission rates in odour units per s ($ou_E\ m^{-3}$ and $ou_E\ s^{-1}$) for well defined sources. One ou_E is the human detection threshold for the odour. Dispersion modelling is frequently undertaken on this basis with odour units being treated in the same way as gases. Guidance is frequently based on the 98^{th} percentile of annual hourly means of odour concentrations although some countries specify the use of higher percentiles in an attempt to account for the importance of short-term peak to mean ratios (e.g. Brancher et al, 2017). The Environment Agency has specified three 'odour benchmarks' of 1.5, 3 and 6 $ou_E\ m^{-3}$ for the most offensive, moderately offensive and less offensive odour types, respectively (Environment Agency, 2011). Odour modelling will be most robust when carried out for elevated point sources with well characterised outputs. However, odours are frequently released from sources with poorly defined emissions which may exhibit a high degree of variability (e.g. fugitive building emissions, low level area sources). In these cases the usefulness of dispersion modelling can be very limited. If there is a possibility of this in the scenario under consideration, discussions should be held with the regulator in advance of undertaking detailed modelling.

A review of odour modelling has recently been commissioned by the ADMLC. For further details, see Price et al. (2021).

A5 Ammonia and Intensive Farming

Ammonia is emitted from intensively farmed livestock and its environmental impact is normally determined for both air concentrations and deposition. At long term concentrations greater than 1 $\mu g\ m^{-3}$ there may be adverse consequences for bryophytes and lichens; at concentrations greater than 3 $\mu g\ m^{-3}$ damage can occur to other, higher forms of vegetation. Ammonia can also contribute to nitrogen and acid deposition. Further information on these processes, UK ammonia background levels and ecological sites can be found on the APIS website (APIS, 2016).

Emission factors from poultry and pig rearing have been determined (Environment Agency, 2012b) and guidance has been provided for an appropriate methodology to be used if detailed modelling is undertaken (Environment Agency, 2010). This takes account of concentration-dependent deposition and plume depletion. Ammonia deposition rates are affected by vegetation type, aerial concentration, time of day and season. Deposition velocities are higher over woodland and also decrease by approximately an order of magnitude over the concentration range 10 – 80 $\mu g\ m^{-3}$.

Detailed guidance on the modelling of non-point sources (of relevance to many ammonia and odour sources) has recently been produced (Stocker et al, 2016).

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