Environment Agency

using science to create a better place

Methods for auditing the contribution of Environment Agency regulated processes to pollution

Science Report: SC030172/SR2

ea/br/e/sci/v1

SCHO0307BMDS-E-P

The Environment Agency is the leading public body protecting and improving the environment in England and Wales.

It is our job to make sure that air, land and water are looked after by everyone in today's society, so that tomorrow's generations inherit a cleaner, healthier world.

Our work includes tackling flooding and pollution incidents, reducing industry's impacts on the environment, cleaning up rivers, coastal waters and contaminated land, and improving wildlife habitats.

This report is the result of research commissioned and funded by the Environment Agency's Science Programme.

Published by:
Environment Agency, Rio House, Waterside Drive, Aztec West,
Almondsbury, Bristol, BS32 4UD
Tel: 01454 624400 Fax: 01454 624409
www.environment-agency.gov.uk

ISBN: 978-1-84432-686-0

This report is printed on Cyclus Print, a 100% recycled stock, which is 100% post consumer waste and is totally chlorine free. Water used is treated and in most cases returned to source in better condition than removed.

Further copies of this report are available from:
The Environment Agency's National Customer Contact Centre by emailing enquiries@environment-agency.gov.uk or by telephoning 08708 506506.

Author(s):
John Abbott, John Stedman and Keith Vincent

Dissemination Status:
Publicly available

Keywords:
Atmospheric dispersion modelling, Lagrangian modelling, transboundary pollution, regional scale, sulphur dioxide, sulphate, dry deposition
Research Contractor:
AEA Technology (Netcen), B551 Harwell, Didcot, Oxfordshire, OX11 0QJ. Tel: 0870 190 6590

Environment Agency's Project Manager:
Bernard Fisher, Kings Meadow House, Reading

Science Project Number:
R&D Project SC030172

Product Code:
SCHO0307BMDS-E-P

Science at the Environment Agency

Science underpins the work of the Environment Agency, by providing an up to date understanding of the world about us, and helping us to develop monitoring tools and techniques to manage our environment as efficiently as possible.

The work of the Science Group is a key ingredient in the partnership between research, policy and operations that enables the Agency to protect and restore our environment.

The Environment Agency's Science Group focuses on five main areas of activity:

- **Setting the agenda**: To identify the strategic science needs of the Agency to inform its advisory and regulatory roles.
- **Sponsoring science**: To fund people and projects in response to the needs identified by the agenda setting.
- **Managing science**: To ensure that each project we fund is fit for purpose and that it is executed according to international scientific standards.
- **Carrying out science**: To undertake the research itself, by those best placed to do it - either by in-house Agency scientists, or by contracting it out to universities, research institutes or consultancies.
- **Providing advice**: To ensure that the knowledge, tools and techniques generated by the science programme are taken up by relevant decision-makers, policy makers and operational staff.

Steve Killeen Head of Science

Executive Summary

This report describes the development of a methodology for the Environment Agency to carry out annual audits for a number of air pollutants for which it has a statutory requirement to regulate emission to air. The methodology builds on the mapping methods currently employed by the National Environmental Technology Centre (Netcen), on behalf of the Department for Environment, Food and Rural Affairs, to produce national scale pollution maps. The Environment Agency can use the annual audits methodology to measure the contribution of sulphur dioxide, oxides of nitrogen and particulate matter to ambient air quality from the processes it regulates, and in particular, its contribution to air quality standards and objectives.

A review of existing mapping methods for sulphur dioxide, oxides of nitrogen and particulate matter identified several areas where improvements could be made. The calibration procedures used to adjust model outputs to available measurements were reviewed, and particular consideration was given to the use of regression analysis and the calculation of prediction intervals and confidence limits.

For sulphur dioxide, a number of improvements and aspects of the mapping methods were investigated. Recent developments in understanding the role played by ammonia in dry deposition were incorporated into long-range transport modelling. A spatial analysis of meteorological data showed that the choice of meteorological station had a relatively small effect on the predicted concentration. The mathematical basis to the addition of background concentrations was provided. For nitrogen dioxide annual mean concentration maps, a nested modelling approach was also adopted. For sulphur dioxide, the models were configured so that there was no double counting of emission data. Because of the diversity of sources of particulate matter, its modelling method was more sophisticated than that carried out for sulphur dioxide or oxides of nitrogen.

The proposed method for each pollutant is presented at the end of this report. This includes recommendations for the choice of input parameters, selection of models, model calibration, sources of emission data, preparation of maps and verification of output.

Contents

1 Introduction

1.1 The Environment Agency's role

The Environment Agency currently regulates the release of pollutants to air in England and Wales from large or complex industrial processes. It also regulates sites where waste is handled such as landfills, composting facilities and fragmentisers. In the future, the Environment Agency will regulate intensive farming and food manufacturing factories. Any of these activities could have a significant effect on air quality.

In carrying out its pollution control functions, the Environment Agency has a statutory responsibility under the Environment Act 1995 to have regard to the government's Air Quality Strategy, including meeting air quality standards and objectives.

The Local Air Quality Management process, which was introduced by Part IV of the Environment Act 1995, places a statutory responsibility on local authorities to review local air quality for seven pollutants. If the objectives for these pollutants are not likely to be met, the local authority must declare a formal Air Quality Management Area and produce an action plan to work towards meeting the air quality objectives. The Environment Agency has an important role to play in this process, as a consultee for local authority reviews and action plans and through the provision of information and the regulation of emissions to air.

The Environment Agency collects annual mass emission data in its Pollution Inventory for over 170 substances released to air from industrial processes regulated under Integrated Pollution Prevention and Control (IPPC). It provides this information to the European Pollutant Emission Register to meet a requirement of the Integrated Pollution Prevention and Control Directive.

The Environment Agency has a statutory responsibility to collect and disseminate information on the state of the environment. It also provides expert advice to government on environmental protection and carries out research on a wide range of environmental issues, including air quality. It comments on the environmental impacts of proposed developments where they may have a significant effect on air quality.

1.2 Annual audits of process contributions to atmospheric pollutant concentrations

An effective way to collect and disseminate information on the state of air quality would be to carry out an annual audit of the contribution to atmospheric pollutant concentrations made by processes regulated by the Environment Agency.

The audit should:

- identify where pollutant concentrations exceed air quality standards and objectives;
- quantify the extent to which air quality standards and objectives are exceeded;
- identify where emissions from Environment Agency-regulated sources make a major contribution to pollutant concentrations;
- quantify the contribution to pollutant concentrations made by Environment Agency-regulated sources;
- identify which source sectors make the greatest contribution to pollutant concentrations.

This report reviews the methods used by the National Environmental Technology Centre (Netcen) to produce concentration maps on behalf of the Department for Environment, Food and Rural

Affairs (Defra), as part of the UK's requirement under EC Directives 96/62/EC and 1999/30/EC. The review then identifies where existing methods should be further developed to provide the most effective means of auditing the contribution from Environment Agency-regulated emissions. Short studies to test the feasibility of suggested amendments to the Netcen method, and research activities forming the basis for the suggested amendments, are described in a series of appendices.

Finally, this report sets out recommended audit methods for each pollutant. A second report will demonstrate the application of these methods to current and future cases.

1.3 Air quality standards and objectives

The Air Quality Regulations 2000, the Air Quality (England) Amendment Regulations 2002 and the Air Quality (Wales) Amendment Regulations 2002 set out air quality objectives for England and Wales. The Air Quality Strategy for England, Scotland, Wales and Northern Ireland: Addendum sets new objectives for particulate matter, PM10. The new objectives for particles are:

- for all parts of the UK, except London and Scotland, a 24-hour mean of 50 µg/m3 not to be exceeded more than seven times per year and an annual mean of 20 µg/m3, both to be achieved by 31 December 2010;

- for Scotland, a 24-hour mean of 50 µg/m3 not to be exceeded more than seven times per year and an annual mean of 18 µg/m3, both to be achieved by 31 December 2010;

- for London, a 24-hour mean of 50 µg/m3 not to be exceeded more than 10 times per year and an annual mean of 23 µg/m3, both to be achieved by 31 December 2010.

These objectives have not been included in the regulations and remain provisional, pending a review by the European Commission of the stage 2 indicative limit value for particles in the first EU Air Quality Daughter Directive, due to be completed by 2004.

The processes regulated by the Environment Agency emit a much wider range of polluting substances than those covered by EU regulations. The Environment Agency has provided a series of long-term (annual average) and short-term (hourly average) Environmental Assessment Levels (EAL) for air as environmental benchmarks for the purpose of Environmental Assessment and Appraisal of BAT for Integrated Pollution Prevention and Control (IPPC). The EAL is the concentration of a substance which, in a particular environmental medium, the regulators regard as a comparator value. It enables a comparison to be made between the environmental effects of different substances in that medium and between environmental effects in different media, along with a summation of those effects.

Table 1.1 summarises these objectives.

In addition to the objectives set out in the Air Quality Regulations, the European Union has set limit values forin respect of nitrogen dioxide and benzene to be achieved by 1 January 2010. The European Union also set limit values for carbon monoxide, sulphur dioxide and lead to be achieved by 2005. Limit values for nitrogen dioxide, sulphur dioxide, carbon monoxide and lead are included in the Air Quality Limit Values Regulations 2003.

Table 1.2 summarises these limit values. The 2003 regulations also include limit values for ozone, but this pollutant is outside the scope of the work in this report.

The Air Quality Strategy for England, Scotland, Wales and Northern Ireland: Addendum sets new objectives for particulate matter, PM_{10}. The new objectives for particles are:

- for all parts of the UK, except London and Scotland, a 24-hour mean of 50 µg/m^3 not to be exceeded more than seven times per year and an annual mean of 20 µg/m^3, both to be achieved by 31 December 2010;
- for Scotland, a 24-hour mean of 50 µg/m^3 not to be exceeded more than seven times per year and an annual mean of 18 µg/m^3, both to be achieved by 31 December 2010;
- for London, a 24-hour mean of 50 µg/m^3 not to be exceeded more than 10 times per year and an annual mean of 23 µg/m^3, both to be achieved by 31 December 2010.

These objectives have not been included in the regulations and remain provisional, pending a review by the European Commission of the stage 2 indicative limit value for particles in the first EU Air Quality Daughter Directive, due to be completed by 2004.

The processes regulated by the Environment Agency emit a much wider range of polluting substances than those covered by EU regulations. The Environment Agency has provided a series of long-term (annual average) and short-term (hourly average) Environmental Assessment Levels (EAL) for air as environmental benchmarks for the purpose of Environmental Assessment and Appraisal of BAT for Integrated Pollution Prevention and Control (IPPC). The EAL is the concentration of a substance which, in a particular environmental medium, the regulators regard as a comparator value. It enables a comparison to be made between the environmental effects of different substances in that medium and between environmental effects in different media, along with a summation of those effects.

Table 1.1: Objectives included in the Air Quality Regulations 2000 and Amendment Regulations 2002 for the purpose of Local Air Quality Management

Pollutant	Air quality objective		Date to be achieved
	Concentration	Measured as	
Benzene			
All authorities	16.25 $\mu g/m^3$	running annual mean	31.12.2003
Authorities in England and Wales only	5.00 $\mu g/m^3$	annual mean	31.12.2010
Authorities in Scotland and Northern Ireland only	3.25 $\mu g/m^3$	running annual mean	31.12.2010
1,3-Butadiene	2.25 $\mu g/m^3$	running annual mean	31.12.2003
Carbon monoxide		maximum daily running eight-hour mean	31.12.2003
Authorities in England, Wales and Northern Ireland only	10.0 mg/m^3		
Authorities in Scotland only	10.0 mg/m^3	running eight-hour mean	31.12.2003
Lead	0.5 $\mu g/m^3$	annual mean	31.12.2004
	0.25 $\mu g/m^3$	annual mean	31.12.2008
Nitrogen dioxide[b]	200 $\mu g/m^3$ not to be exceeded more than 18 times a year	one-hour mean	31.12.2005
	40 $\mu g/m^3$	annual mean	31.12.2005
Particles (PM_{10}) (gravimetric)[c] All authorities	50 $\mu g/m^3$ not to be exceeded more than 35 times a year	24-hour mean	31.12.2004
	40 $\mu g/m^3$	annual mean	31.12.2004
Authorities in Scotland only[d]	50 $\mu g/m^3$ not to be exceeded more than seven times a year	24-hour mean	31.12.2010
	18 $\mu g/m^3$	annual mean	31.12.2010
Sulphur dioxide	350 $\mu g/m^3$ not to be exceeded more than 24 times a year	one-hour mean	31.12.2004
	125 $\mu g/m^3$ not to be exceeded more than three times a year	24-hour mean	31.12.2004
	266 $\mu g/m^3$ not to be exceeded more than 35 times a year	15-minute mean	31.12.2005

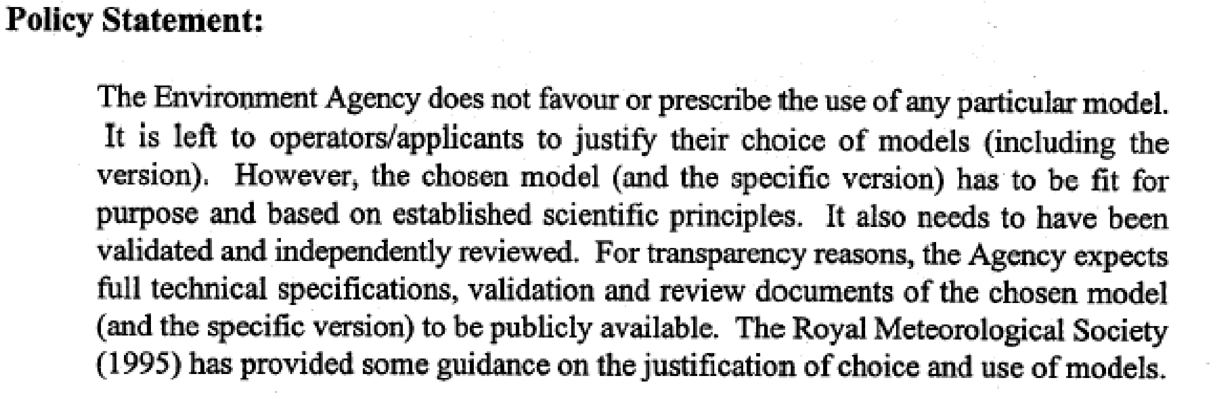
b. The objectives for nitrogen dioxide are provisional.
c. Measured using the European gravimetric transfer standard sampler or equivalent.
d. These 2010 Air Quality Objectives for PM10 apply in Scotland only, as set out in the Air Quality (Scotland) Amendment Regulations 2002.

Table 1.2: Air quality limit values in the Air Quality Limit Values Regulations 2003

Pollutant	Air quality objective		Date to be achieved
	Concentration	**Measured as**	
Benzene			
Limit value for the protection of human health	5.00 µg/m^3	annual mean	1.1.2010
Carbon monoxide Limit value for the protection of human health	10.0 mg/m^3	maximum daily running eight-hour mean	1.1.2005
Lead			
Annual limit value for the protection of human health	0.5 µg/m^3	annual mean	1.1.2005
Nitrogen dioxide			1.1.2010
Hourly limit value for the protection of human health	200 µg/m^3 not to be exceeded more than 18 times a year	one-hour mean	
Annual limit value for the protection of human health	40 µg/m^3	annual mean	1.1.2010
Oxides of nitrogen			
Annual limit value for the protection of vegetation	30 µg/m^3	annual mean	19.7.2001
Particles (PM_{10}) (gravimetric)[c]			
24-hour limit value for the protection of human health	50 µg/m^3 not to be exceeded more than 35 times a year	24-hour mean	1.1.2005
Annual limit value for the protection of human health	40 µg/m^3	annual mean	1.1.2005
Sulphur dioxide			
Hourly limit value for the protection of human health	350 µg/m^3 not to be exceeded more than 24 times a year	one-hour mean	1.1.2005
Daily limit value for the protection of human health	125 µg/m^3 not to be exceeded more than three times a year	24-hour mean	1.1.2005
Annual limit value for the protection of ecosystems	20 µg/m^3	annual mean	19.7.2001
Winter limit value for the protection of ecosystems	20 µg/m^3	winter mean (1st October to 31 st March)	19.7.2001

1.4 Environment Agency guidance on the use of dispersion models

Dispersion models form an integral part of the methods used to prepare pollutant concentration maps as part of the audit process. The Environment Agency has prepared a policy statement on how dispersion models should be selected: (http://www.environment-agency.gov.uk/commondata/105385/eas200711.pdf):



Policy Statement:

> The Environment Agency does not favour or prescribe the use of any particular model. It is left to operators/applicants to justify their choice of models (including the version). However, the chosen model (and the 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 some guidance on the justification of choice and use of models.

To summarise, the choice of model must be:

- fit for purpose;
- based on established scientific principles;
- validated and independently reviewed;
- have full technical specifications, validation and review documents which must be available.

The recommendations for an annual audit methodology in this report are intended to be applicable to any dispersion models that meet these requirements. However, the methodology has been developed using two specific dispersion models, ADMS Version 3.1 for short-range impacts and TRACK 1.7 for long-range impacts.

ADMS 3.1 has been widely used for the assessment of short-range impact pollutant emissions. The developers, Cambridge Environmental Consultants (CERC), maintain a website (http://www.cerc.co.uk/software/publications.htm) that provides details of technical specifications and validation studies.

The technical specification for the TRACK model is described in a refereed paper by Lee *et al.* (2000). More recently, predictions of deposition rates and ambient concentrations made by Version 1.7 have been compared with measured values by Abbott *et al.* (2003). Verification of model predictions against available measurements of pollutant concentrations is a fundamental feature of the audit methodology recommended in this report.

The Environment Agency also provides guidance on the reporting of detailed dispersion modelling studies. (http://www.environment-agency.gov.uk/commondata/105385/report_edited_252797.pdf) The audit methodology recommended in this report provides further guidance on the reporting of dispersion modelling studies for national/annual audit purposes.

2 Overview of methods used by Netcen to produce pollutant concentration maps for Defra

Netcen has produced concentration maps for sulphur dioxide, nitrogen dioxide and particulate matter, PM_{10} on behalf of Defra for the years 2001 and 2002, as part of the UK's obligation under EC Directives 96/62/EC and 1999/30/EC. This work provides a starting point for the development of an audit methodology for the Environment Agency.

The methods used for each pollutant differ slightly. However, the general procedure is similar in each case. The contributions to pollutant concentrations from large industrial sources, small industrial sources and other sources of domestic and transport emissions are determined separately by means of dispersion modelling. Other residual contributions are then estimated by analysing monitoring data. Full details of the modelling methods used are given in the sections below. A brief introduction is presented here. Maps of background concentrations of SO_2, NO_2 and PM_{10} have been prepared on a 1 km x 1 km grid for the 2002 calendar year. Maps of roadside concentrations of NO_2 and PM_{10} have also been prepared for 9,360 built-up major road links (A-roads and motorways).

There are many similarities between the methods used for each pollutant. However, there are also subtle differences. The detailed descriptions of the methods in the following sections contain some repetition between pollutants.

Dominant contributions to SO_2 concentrations in the UK are typically from major point sources such as power stations and refineries, particularly in terms of high percentile concentrations. Emissions of SO_2 from point sources were therefore modelled explicitly in some detail. Domestic, transport and small industrial sources were modelled in less detail on the basis of the National Atmospheric Emission Inventory, a 1 km x 1 km disaggregated inventory, using a dispersion kernel approach. A dispersion kernel describes the contributions to ambient concentrations of a pollutant at a central receptor location, from each of a regular array of sources of unit emission strength. Measured SO_2 concentrations from rural SO_2 monitoring network (Hasler *et al.,* 2001) sites, rural, suburban and industrial sites in the national automatic monitoring networks and rural automatic monitoring sites maintained by electricity generating companies were used to calibrate the SO_2 model output. The residual contribution to ambient annual mean concentrations from sources not modelled was estimated from the measurements, corrected for the contributions to concentrations at these locations from modelled sources.

For NO_2, NO_x and PM_{10}, traffic sources make an important contribution to ambient concentrations in urban areas. The calibration procedure therefore takes measurements made at urban background monitoring sites into account. Roadside concentrations of NO_2, NO_x and PM_{10} were estimated by adding a roadside increment to the modelled background concentrations. The roadside increment was calculated from road link emission estimates, using dispersion coefficients derived empirically using data from roadside monitoring sites.

3 Netcen method for sulphur dioxide

Netcen have prepared national scale maps of sulphur dioxide concentrations for comparison with the air quality objectives and limit values presented in Table 3.1.

Table 3.1: Air quality limit values and objectives for sulphur dioxide

Pollutant	Air quality objective or limit value		Date to be achieved by
Sulphur dioxide	350 $\mu g/m^3$ not to be exceeded more than 24 times a year	one-hour mean	31.12.2004
	125 $\mu g/m^3$ not to be exceeded more than three times a year	24-hour mean	31.12.2004
	266 $\mu g/m^3$ not to be exceeded more than 35 times a year	15-minute mean	31.12.2005
Annual limit value for the protection of ecosystems	20 $\mu g/m^3$	annual mean	19.7.2001
Winter limit value for the protection of ecosystems	20 $\mu g/m^3$	winter mean (1st October to 31 st March)	19.7.2001

3.1 Emissions estimates and discharge conditions

All Part A processes in the National Atmospheric Emission Inventory (NAEI) with emissions greater than 500 tonnes per annum were included in the detailed dispersion modelling study.

The following parameters were used to characterise the emissions from each of the modelled Part A processes:

- emission rate;
- stack height;
- stack diameter;
- discharge velocity;
- discharge temperature.

Emissions data were taken from the NAEI based on reported emissions in the Environment Agency's Chemical Release Inventory.

Environment Agency regional offices were contacted and asked to provide details of the discharge conditions from Part A sources in each region. The information provided was used in the modelling study, and supplemented with details taken from the IPC authorisations and IPPC permit applications. Other information was obtained from recent modelling studies carried out at Netcen. Where no information was available on discharge conditions, best engineering judgements were made on suitable estimates. The judgements included consideration of the likely sulphur content and calorific values of the fuel used in order to estimate discharge velocities and the heat content of the discharging plume, and use of HMIP's Technical Guidance Note D1 to estimate stack heights.

Many Part A processes emit sulphur dioxide through multiple stacks. We have ignored the possible enhancement of plume rise that may occur when plumes combine from stacks located near to each other. Where there are many stacks at the same site with different discharge conditions, for example at refineries or chemical works, we have, in some cases, grouped stacks of similar height and discharge characteristics together. We have then assumed that the emission from each group of stacks may be represented by a single stack with characteristics of the stack with the largest emission, or by a stack with an emission-weighted ‘average’ stack.

Appendix 1 lists the emission rates and discharge characteristics used for modelling 2003 sulphur dioxide emissions.

Power stations do not produce electricity at a constant rate, with electricity generation increasing and decreasing with demand. A default demand profile has been assumed for each of the coal-fired power stations operating in the UK, based on data provided by the National Grid Company and contained with the company’s Seven Year Statement for 1998. The statement sets out the amount of electricity generated by a large coal plant for typical winter and summer days in the United Kingdom, together with the total electricity generating capacity for a large coal plant (18.67 GW).

Typical load factors shown in Table 3.2 were derived by dividing the electricity generated in each period by the total generating capacity. Scaling factors were then derived for each hour of the year to relate hourly average emission rates to the annual average emission rate. These are shown in

Table 3.3. For example, the hourly emission rate starting at 16:00 during the winter period for a plant emitting 60,000 tonnes of sulphur dioxide per year, corresponding to an average emission rate of 1,902 g s^{-1}, was 1.69 x 1,902 = 3,215 g s^{-1}. The summer scaling factors were applied from 2 March to 31 August and the winter scaling factors were applied during the rest of the year. The discharge volumetric flow rate from the stack was also scaled in the same way.

Table 3.2: Average load factors

Time	Electricity generated from large coal combustion, GW		Load factor	
	Winter	**Summer**	**Winter**	**Summer**
22 to 5	8.43	4.06	0.45	0.22
6 to 9	13.57	10.15	0.73	0.54
10 to 12	16.07	11.58	0.86	0.62
13 to 15	16.00	11.55	0.86	0.62
16 to 18	18.15	10.02	0.97	0.54
19 to 21	14.84	8.45	0.79	0.45

Note: the total generating capacity from a large coal plant is 18.67 GW

Table 3.3: Scaling factors to relate hourly average emission rates to the annual average emission rate.

		Winter	Summer
Scaling factors for each hour of the year	22 to 5	0.79	0.38
	6 to 9	1.27	0.95
	10 to 12	1.50	1.08
	13 to 15	1.49	1.08
	16 to 18	1.69	0.93
	19 to 21	1.38	0.79

Emissions from smaller industrial sources regulated by the Environment Agency with emissions of less than 500 tonnes per annum were obtained from the NAEI on a 1 km x 1 km basis. The NAEI provides no details of the discharge conditions from these smaller industrial sources of sulphur dioxide emissions. It was therefore assumed that the discharge height meets the requirements of the Chimney Heights Memorandum, 3rd edition. Other assumptions included a discharge temperature of 100°C, a discharge velocity of 10 m s^{-1} and a sulphur dioxide concentration in the discharge of 3,000 mg m^{-3} at reference conditions. Further details are provided in Appendix 2.

Estimates of emissions from domestic, transport, Part B industrial sources and other area sources were obtained from the NAEI for each one km square area. Emissions from each source were assumed to be distributed uniformly through an initial height of 10 m: that is, each one km source was represented by an emitting volume 1 km x 1 km square and 10 m high. The estimate of 10 m is based on the height of a typical house and assumes that emissions will be entrained in the building wake.

3.2 Dispersion modelling

Netcen uses the dispersion model, ADMS Version 3.1, to calculate sulphur dioxide concentrations. Contributions from large industrial sources, small industrial sources and other area sources were modelled separately: the methods used are described below. The procedure used to calculate high percentile sulphur dioxide concentrations in urban areas of Northern Ireland is different from that employed for the rest of the United Kingdom, because emissions from domestic combustion of solid fuels is of particular concern there. The empirical procedure is not described here because it is not applicable in England and Wales (the area regulated by the Environment Agency), but it is described elsewhere (Stedman *et al.,* 2002).

3.2.1 Large industrial sources

A number of receptor areas which together cover most of the UK were defined for the purposes of modelling the contribution to sulphur dioxide concentrations from large industrial sources. Each receptor area was 100 km square, extending out to 150 km to cover coastal areas where appropriate (Figure 3.1). All sources within the receptor area and sources in the adjoining 100 km square areas were included when modelling the combined effect of Part A sources on the concentration in the receptor area. Concentrations were calculated on a regular five km grid throughout the receptor areas.

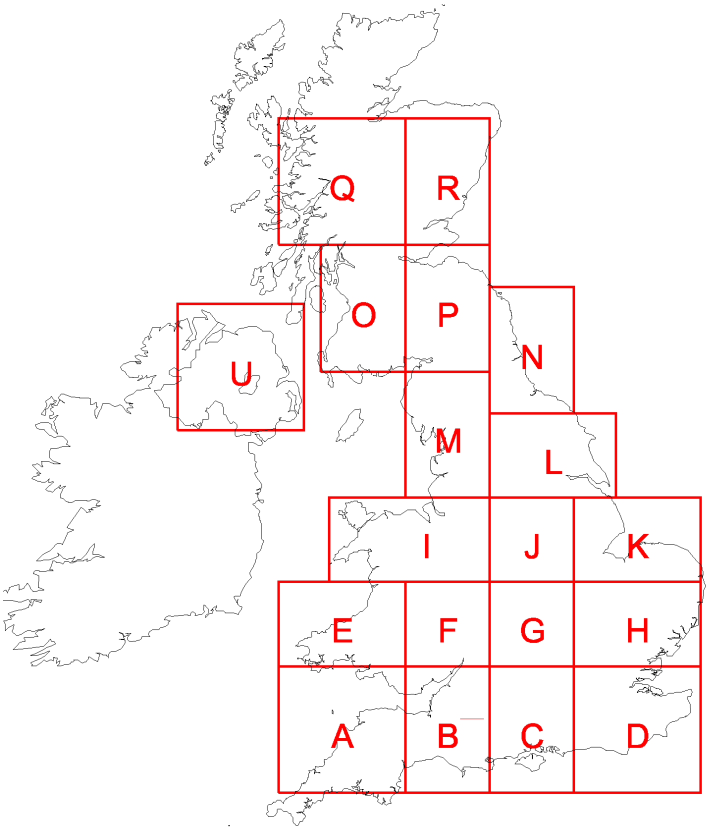


Figure 3.1: Receptor areas defined for modelling the contribution of sulphur dioxide from large industrial sources

Various data sets have been used to represent meteorological conditions. Most recently, sequential hourly data from Waddington for 2002 and 2003 obtained from the Meteorological Office has been used to represent meteorological conditions throughout the whole country for the appropriate year. This was used for the purposes of modelling the contribution from large Part A processes. The sequential data provides hourly information of windspeed, wind direction, cloud cover, relative humidity and precipitation. A uniform surface roughness of 0.1 m, typical of agricultural areas, was used for the whole country. A wet and dry deposition has usually not been taken into account in the most recent Netcen assessments, although a dry deposition velocity of 0.01 m/s was assumed in earlier assessments. Wet deposition has not been taken into account.

3.2.2 Area sources

The annual average contribution from area sources other than small Part A industrial sources was calculated on a one km receptor grid covering the country, using the dispersion model ADMS Version 3.1. Each source was represented as a volume source 10 m high and one km square. Contributions at each receptor from sources at distances greater than 15 km in the north-south or east-west directions were ignored. The calculation was facilitated by means of a dispersion kernel approach. A dispersion kernel describes the contributions to ambient concentrations of a pollutant at a central receptor location from each of a regular array of sources of unit emission strength. The dispersion kernel is derived as follows:

1. Use ADMS 3.1 to model the contribution from a unit source area centred on (0, 0) to receptors on a regular 1 km x 1 km grid extending from (–15000, -15000 m) to (15000, 15000 m).
2. Note that, for flat terrain and uniform meteorology, the contribution from a source at (0, 0) to a receptor at (a, b) is the same as the contribution from an equivalent source at (–a,-b) to a receptor at (0, 0). Multiply the x and y coordinates by –1 to derive the dispersion kernel.

The dispersion kernel is used as a weighting function so that the concentration $c_{l,m}$ (μg m^{-3}) at a receptor at l,m is given by:

$$c_{l,m} = \sum_{i=-15}^{15} \sum_{j=-15}^{15} k_{i,j} e_{l+i,m+j}$$

where $k_{i,j}$ are the elements of the dispersion kernel ((μg m^{-3})/(g/s)) and $e_{l,m}$ are the emission rates (g/s) for each grid square.

A uniform surface roughness of one metre, corresponding to typical urban areas, was used for the whole country. Wet and dry deposition were ignored. Various data sets have been used to represent meteorological conditions. Most recently, sequential hourly data from Waddington for 2002 and 2003 obtained from the Meteorological Office has been used to represent meteorological conditions throughout the whole country (except the London area) for the appropriate year. Similar meteorological data for Heathrow have been used for the London area.

An upper limit of 2 μg m^{-3} was applied to the area source contribution from the 'other transport' source sector (mostly shipping).

A similar approach has been used for small industrial sources regulated by the Environment Agency. However, a non-linear correction factor was used to take account of stack height, plume momentum and buoyancy effects from point sources:

$$c_{l,m} = \sum_{i=-15}^{15} \sum_{j=-15}^{15} k_{i,j}.10.\left(\frac{e_{l+i,m+j}}{10}\right)^{2/3}$$

An in-square contribution from small point sources was also calculated, because the point source is unlikely to be located at the centre of the grid square:

$$c_{l,m} = 1.98 e_{l,m}^{0.5}$$

The derivation of these empirical adjustments is provided in Appendix 2.

3.2.3 Addition of modelled contributions to sulphur dioxide concentrations

Dispersion modelling carried out by Netcen provides modelled estimates of the following contributions to sulphur dioxide concentrations:

- annual average contribution from large industrial sources;
- 99.9th percentile of 15-minute averages of the contribution from the large sources;
- 99.73th percentile of one-hour averages of the contribution from the large sources;
- 99.18th percentile of 24-hour averages of the contribution from the large sources;
- annual average contribution from small industrial sources;
- annual average contribution from other area sources.

To assess the impact of emissions from industrial sources on local air quality using dispersion models, it is necessary to predict the contribution of the industrial source to ground level concentrations and then add the predicted contribution to background concentrations from other sources. For sulphur dioxide, the impact of air quality on ecosystems is assessed in terms of pollutant concentrations averaged over a year or winter period: the total concentration is simply the sum of the source and background averaged component concentrations. However, the effects of sulphur dioxide on human health are set in terms of the highest percentiles of hourly, daily and 15-minute averaged concentrations experienced in a year. For impacts assessed in this way, it is not appropriate to add the high percentile modelled contributions to the high percentile background concentrations, because the peak concentrations may not occur at the same time.

This problem is particularly marked for emissions from large industrial sources, because the meteorological conditions that produce high concentrations from tall stacks are not the same as those that produce the highest concentrations from emissions at low level. Abbott and Downing (2000) carried out modelling studies to assess the accuracy of a range of simple methods for adding background concentrations. This assessment indicated that the total percentile concentration may be assessed as the larger of: a) the modelled percentile contribution from the industrial source plus twice the annual mean from low-level sources; or b) the modelled percentile contribution from the low-level sources plus twice the annual mean from the industrial sources. Further studies for the Environment Agency are currently in progress.

The Netcen method for producing national maps adds the modelled high percentile contribution from the large industrial sources to a multiple of the annual mean background from other sources. For the 99.9th percentile 15-minute average and the 99.73th percentile of hourly means the multiplier is two, while for other metrics the multiplier is unity.

3.3 Model calibration

Measured SO_2 concentrations at monitoring sites across the United Kingdom were used to calibrate the SO_2 model output, to ensure that final predicted concentrations matched the concentrations measured at these sites. Data from rural, suburban and industrial sites in the national automatic monitoring networks and rural automatic monitoring sites maintained by electricity generating companies were used to calibrate the model for the prediction of the percentile sulphur dioxide concentrations. Sites with data capture of less than 75 per cent were excluded from the analysis. The continuous automatic monitoring data was supplemented with data from the rural SO_2 monitoring network (Hasler *et al*., 2001) sites for the calibration of the annual average model. A list of sites is included in Appendix 3.

Urban background, urban centre, urban industrial and roadside sites within the automatic monitoring networks, and those operated on behalf of local authorities but not in the national network, were not included in the calibration because emission sources of sulphur dioxide are not well characterised in these areas. For example, the information available from the NAEI at a 1 km x 1 km level is insufficiently detailed to characterise domestic emissions at the level of fuel use within individual housing estates. Small industrial sources may affect the concentrations measured in urban areas, but are accounted for in detail in the national scale model.

The calibration was based on a regression model of the form:

$$c_{measured} = Ac_{\mathrm{mod}elled\_industrial} + B + mc_{\mathrm{mod}elled\_area}$$

where m is a background multiplier factor (see 3.2.3)
A is a constant determined by the regression analysis

B is a constant variously determined by the regression analysis or on the basis of a priori judgement.

Figure 3.2 shows a graph of the regression model predictions of annual mean concentrations for 2002 plotted against the observed concentrations (A = 0.905, B = -0.15 μg m^{-3}, m = 1). Figure 3.3 shows a graph of the regression model predictions of 99.18th percentile of daily mean concentrations for 2002 plotted against the observed concentrations (A = 1.20, B = 5 μg m^{-3}, m = 1). Figure 3.4 shows a graph of the regression model predictions of 99.73th percentile of daily mean concentrations for 2002 plotted against the observed concentrations (A = 1.05, B = 4 μg m^{-3}, m = 2).

Figure 3.5 shows a graph of the regression model predictions of 99.9th percentile of 15-minute mean concentrations for 2003 plotted against the observed concentrations (A = 1.10, B = 20 μg m^{-3}, m = 2).

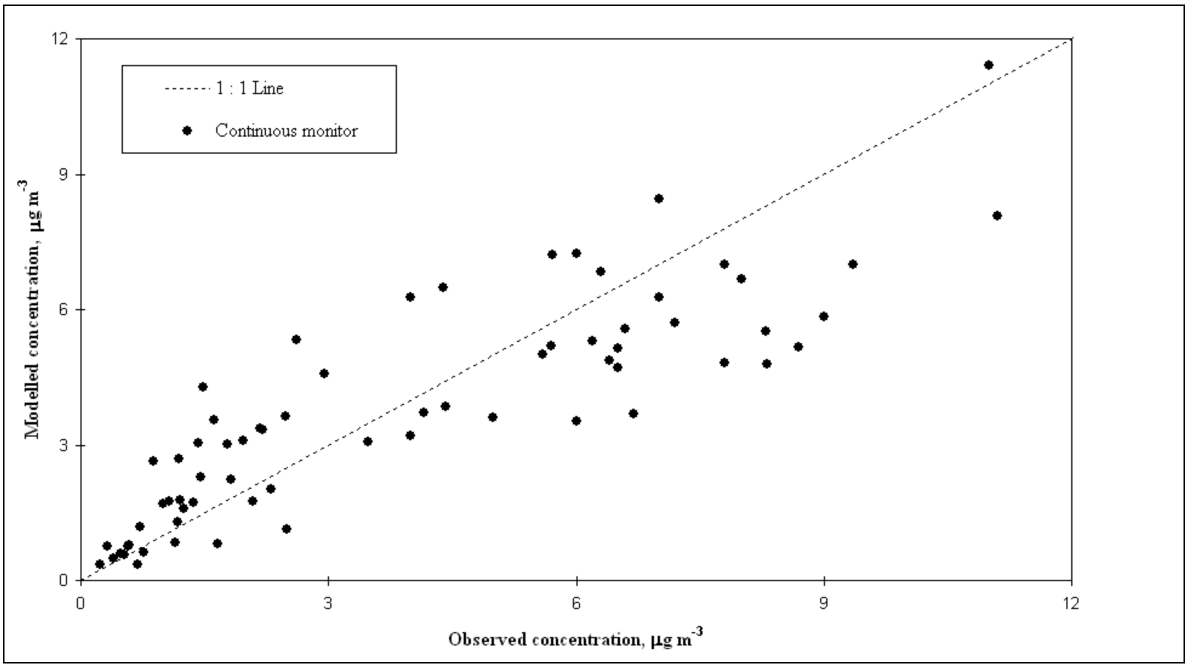


Figure 3.2: Calibration plot for 2002 annual mean SO_2 concentration

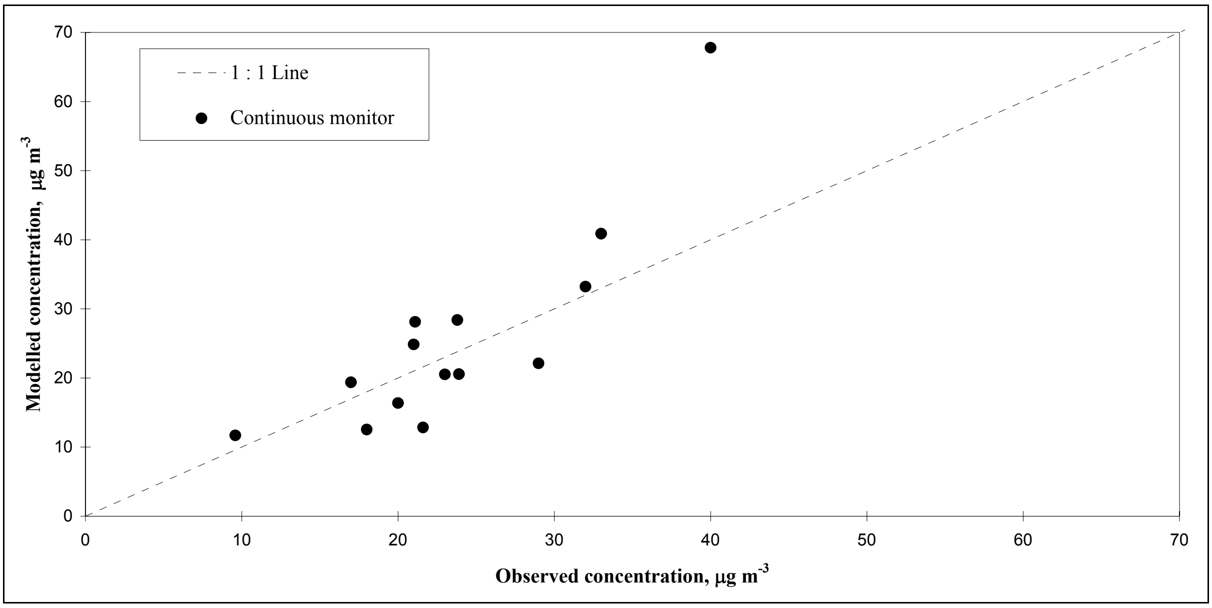


Figure 3.3: Calibration plot for 2002 99.18th percentile of 24-hour mean SO_2 concentrations

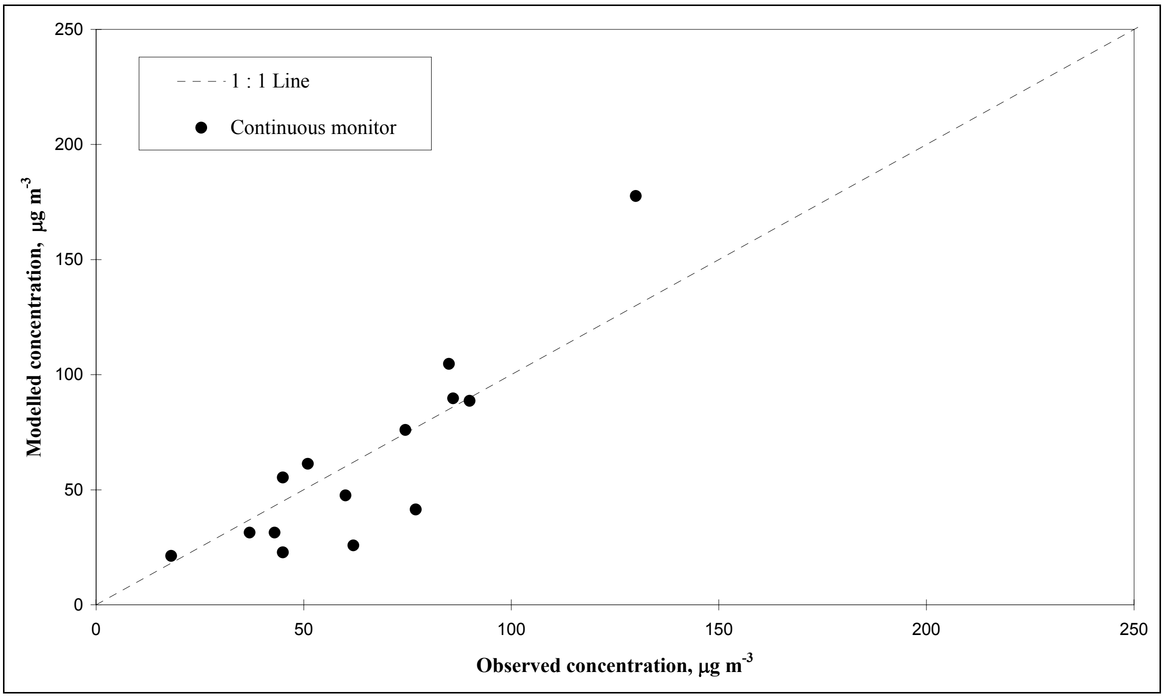


Figure 3.4: Calibration plot for 2002 99.73th percentile of 24-hour mean SO_2 concentrations

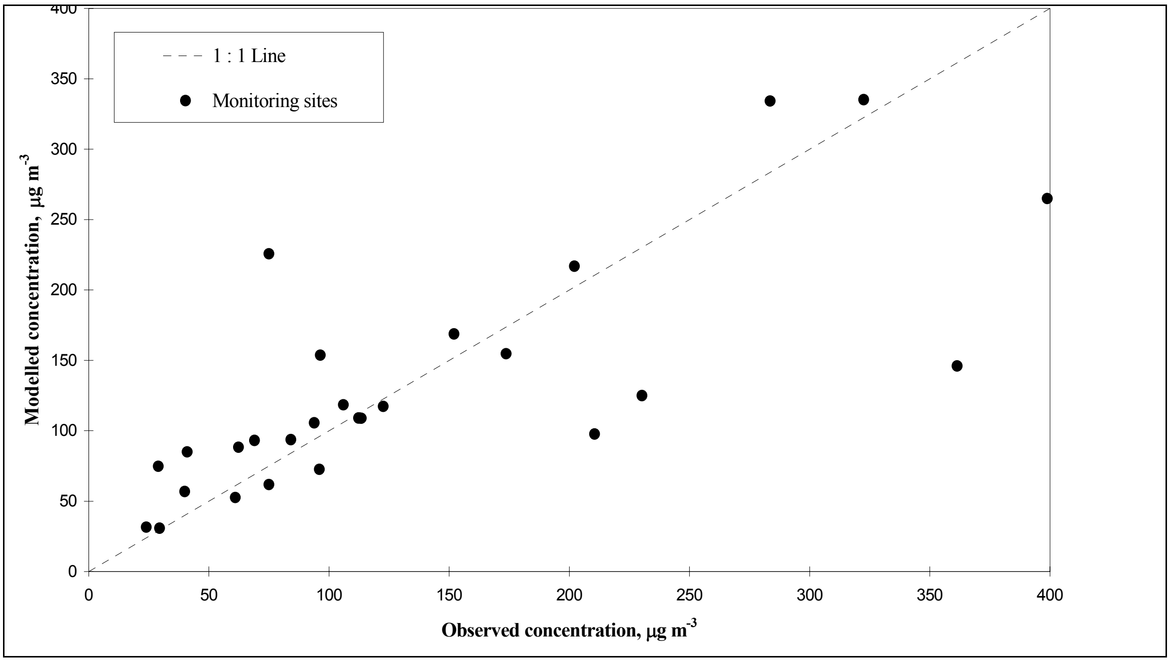


Figure 3.5: Calibration plot for 2003 99.9th percentile of 15-minute mean SO_2 concentrations

Residual concentrations were then calculated at each of the calibration monitoring sites:

Residual = measured - regression model

These residual contributions are associated partly with errors in the model and partly with the contributions from more distant sources, not modelled in this study. They include, for example, contributions from emissions from sources on continental Europe. The residual concentrations were interpolated across the country to provide a map of residuals using simple kriging using the Surfer^{TM} contouring software. The final map was calculated from:

Mapped value = regression model + residual

This procedure forces the mapped value to equal the measured value at each of the calibration sites. It is recognised that this 'corset fitting' procedure introduces equivalent errors at other locations.

It was not possible to calibrate the area source model using sulphur dioxide monitoring data because the 1 km x 1 km disaggregated emission data was not sufficiently detailed or accurate. However, the emission inventory for oxides of nitrogen was better because the major part of the emission in urban areas is associated with road traffic which is quantified in greater detail. The performance of the 1 km x 1 km area source dispersion model was therefore assessed by comparing modelled and measured oxides of nitrogen concentrations. Figure 3.6 shows a scatter plot of modelled and measured oxides of nitrogen concentrations. Further details of the assessment are reported elsewhere (Coleman *et al.*, 2001). The model was applied to sulphur dioxide emissions without calibration on the basis of its performance for oxides of nitrogen.

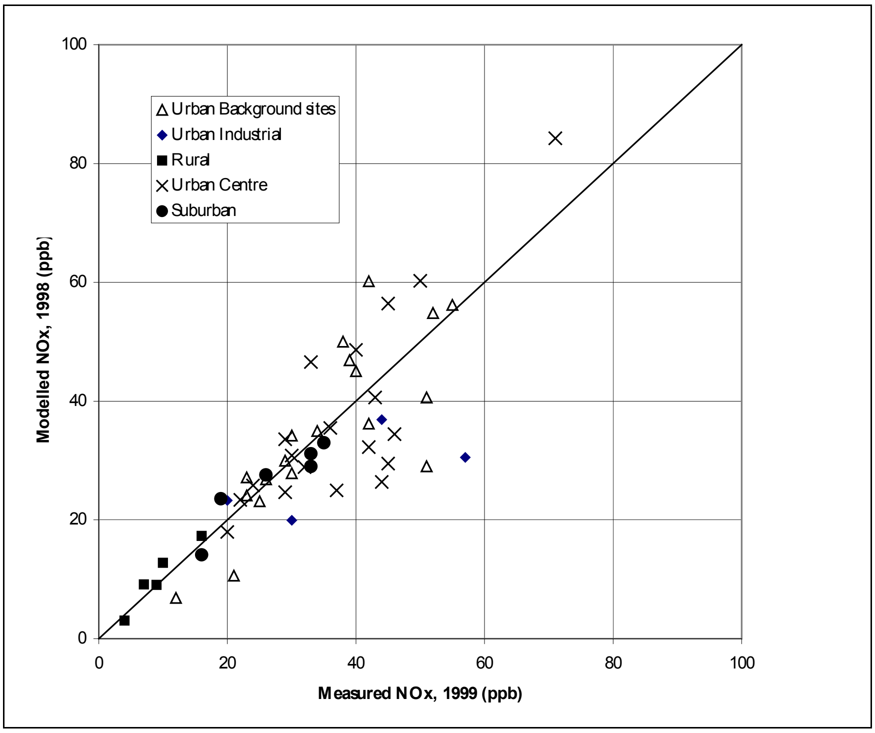


Figure 3.6: A scatter plot of modelled and measured oxides of nitrogen concentrations

3.4 Model verification

Concentrations predicted by the regression model were then compared with measured values at the urban background and urban centre sites within the automatic monitoring networks excluded from the calibration. The purpose of this verification was to assess the performance of the model in urban areas. Model performance was likely to be relatively poor in these areas, because information available from the NAEI at a 1 km x 1 km level is insufficiently detailed to characterise domestic emissions from fuel use within individual housing estates, and because small industrial sources may affect levels measured in urban areas without being accounted for in the national scale model.

Figure 3.7, Figure 3.8 and Figure 3.9 show the verification plots for 2003 for the 99.73th percentile hourly average, 99.18th percentile 24-hour average and the 99.9th percentile 15-minute average concentrations, respectively. In each case, the model underestimates the measured concentrations at sites in Barnsley and Tameside, where there may be significant local domestic emissions. The model overestimates the measured concentrations in Port Talbot.

Figure 3.10 shows the verification plot for 2003 for the annual average concentration. The plot shows that the model does not provide satisfactory estimates of annual average concentrations in urban areas. However, the annual average limit value for sulphur dioxide has been set for the protection of ecosystems and does not apply in urban areas. Consequently, the model is not required to assess annual average concentrations in urban areas.

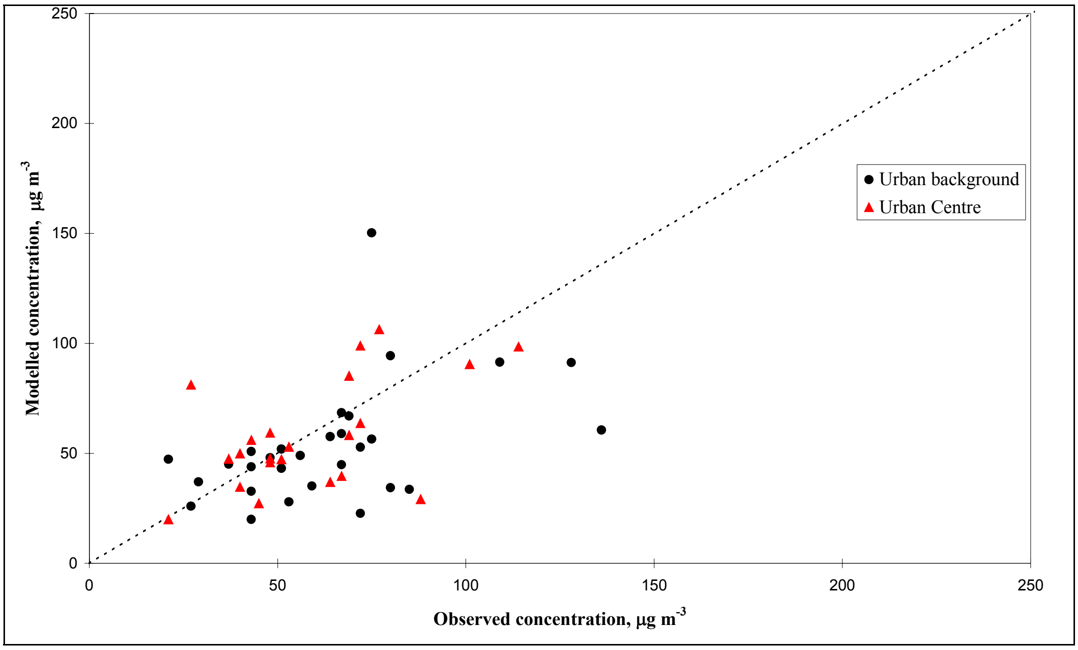


Figure 3.7: Verification plot of modelled 99.73th percentile hourly average SO_2 concentrations 2003 at urban centre and urban background sites (excluding Northern Ireland)

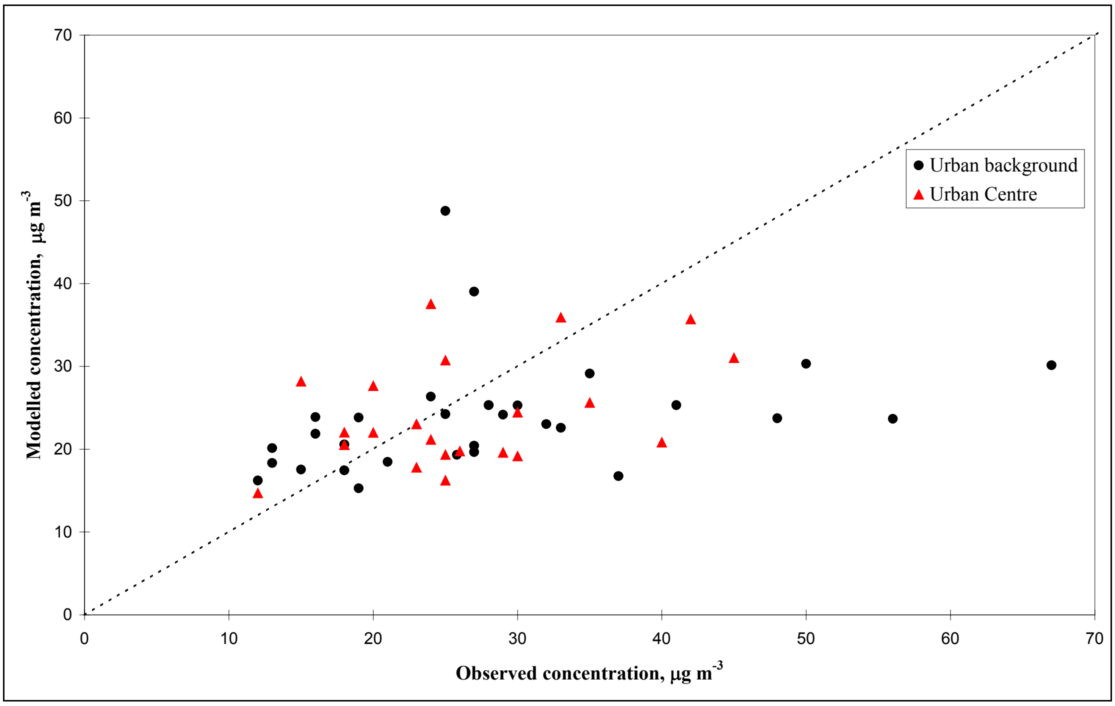


Figure 3.8: Verification plot of modelled 99.18th percentile 24-hour average SO_2 concentrations 2003 at urban centre and urban background sites (excluding Northern Ireland)

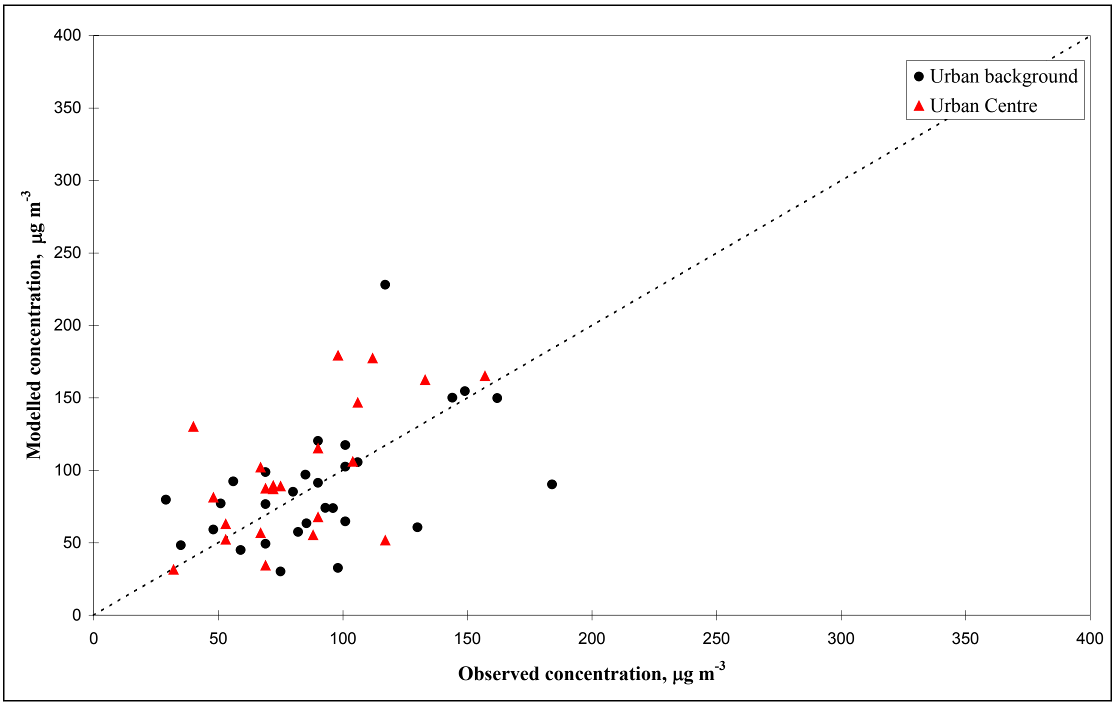


Figure 3.9: Verification plot of modelled 99.9th percentile 15-minute average concentrations 2003 at urban centre and urban background sites (excluding Northern Ireland)

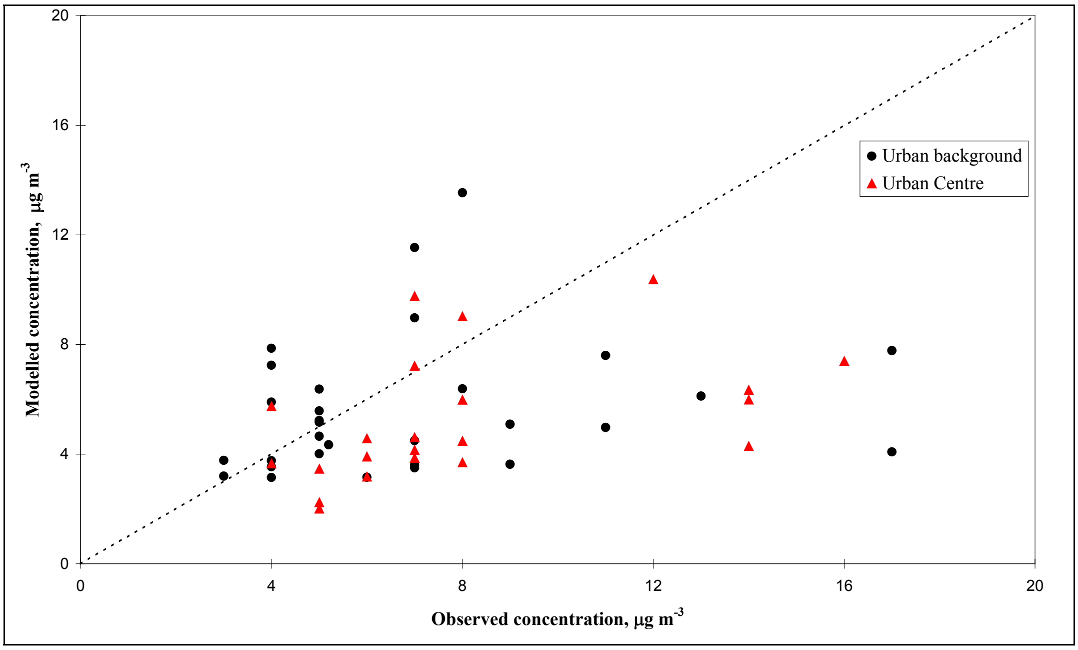


Figure 3.10: Verification plot of modelled annual average concentrations 2003 at urban centre and urban background sites (excluding Northern Ireland)

3.5 Preparation of maps

Netcen currently prepare the required maps using the Geographical Information System ArcInfo, which was used here. Simple scripts were prepared in the ArcInfo command language (*.aml) to facilitate the data handling operations.

Figure 3.11 shows the predicted annual average concentrations for 2002. A data mask was applied in ArcInfo to exclude those areas where the annual average limit value for sulphur dioxide did not apply. This mask was based on urban agglomerations, other urban areas, and distance from road links and industrial plant.

Agglomerations in England were based on the Ordnance National Survey data set for urban areas and settlement boundaries. For Scotland and Northern Ireland, the Scottish Executive Urban Rural Classification and the Belfast Metropolitan Urban Areas were used, respectively. For each of these areas an additional 20 km buffer area was applied. A five km buffer was applied around the other urban areas, road links and Part A authorised processes.

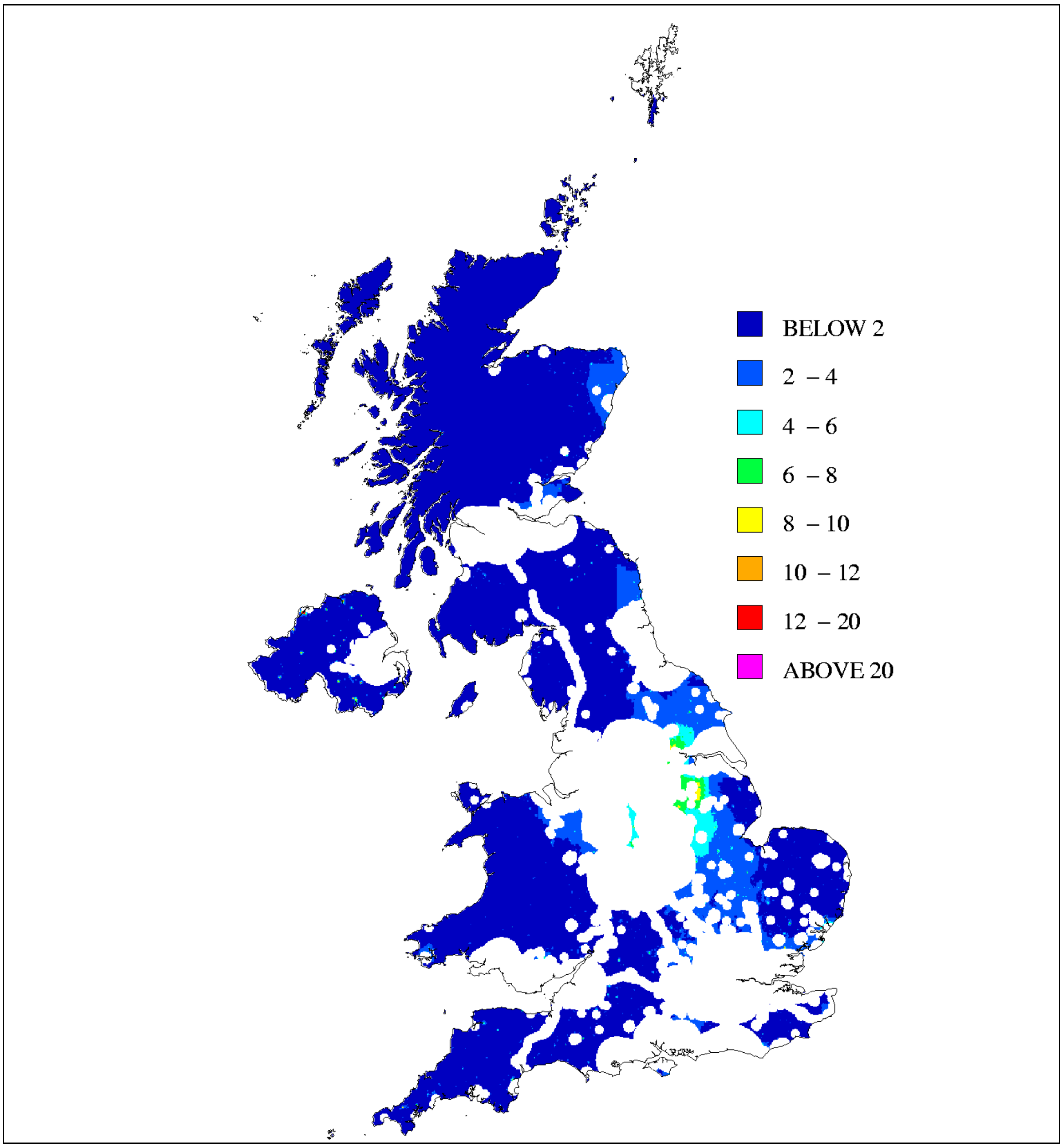


Figure 3.11: Annual average SO_2 concentrations for 2002. Concentrations are predicted for 1 km x 1 km squares.

A map of winter mean SO_2 concentrations for the period October 2001 to March 2002 was also calculated and is shown in Figure 3.12. This map was calculated by multiplying the annual mean map for 2002 by 1.16, the average ratio between the 2001-2002 winter and 2002 annual means measured at rural SO_2 monitoring sites (Hasler *et al.*, 2001).

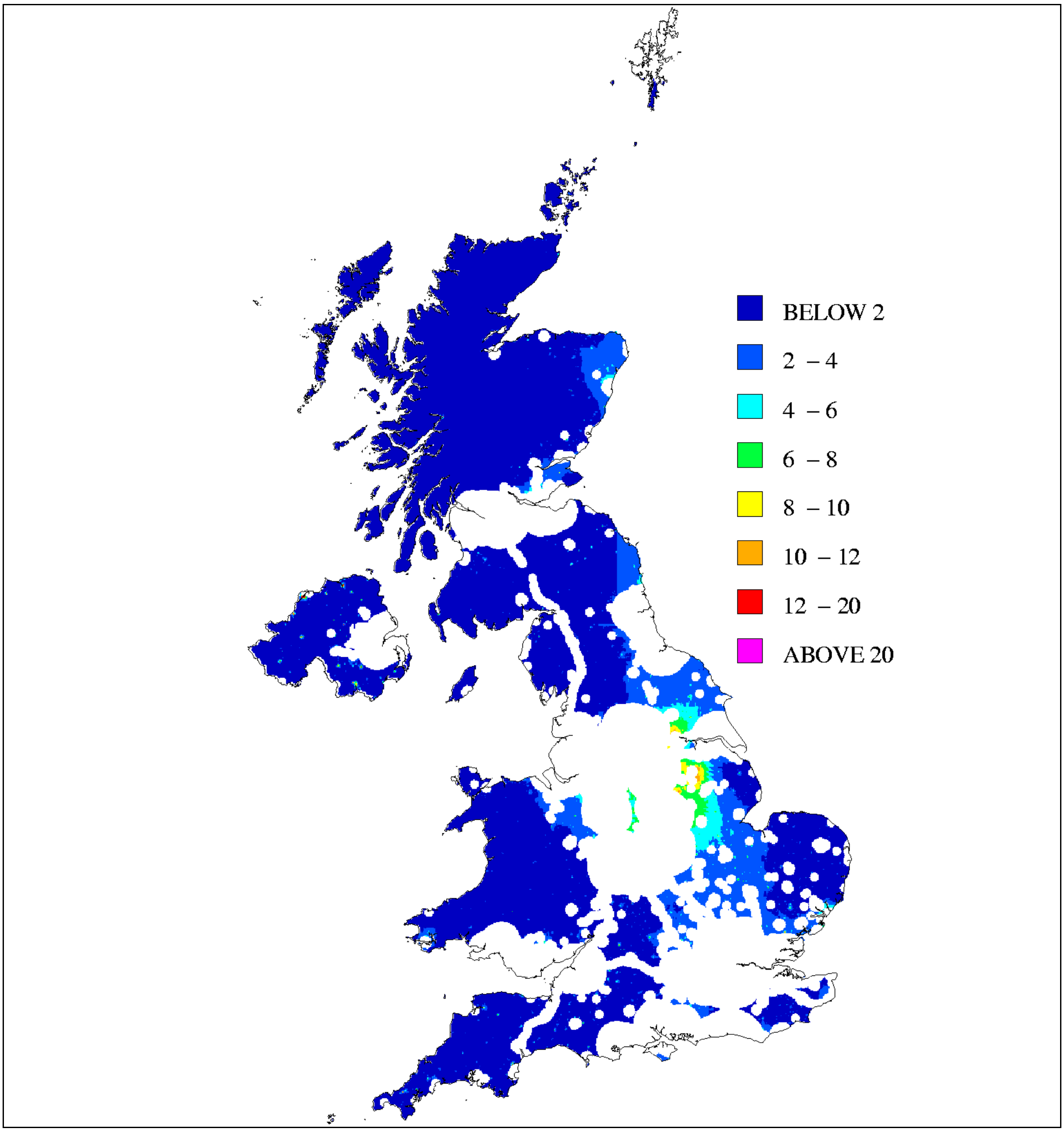


Figure 3.12: Winter mean SO_2 concentrations 2001-2002 ($\mu g\ m^{-3}$) in ecosystem areas. Concentrations are predicted for 1 km x 1 km squares.

A map of the 99.73th percentile of one-hour means in 2002 is shown in Figure 3.13 for comparison with the one-hour limit value for SO_2.

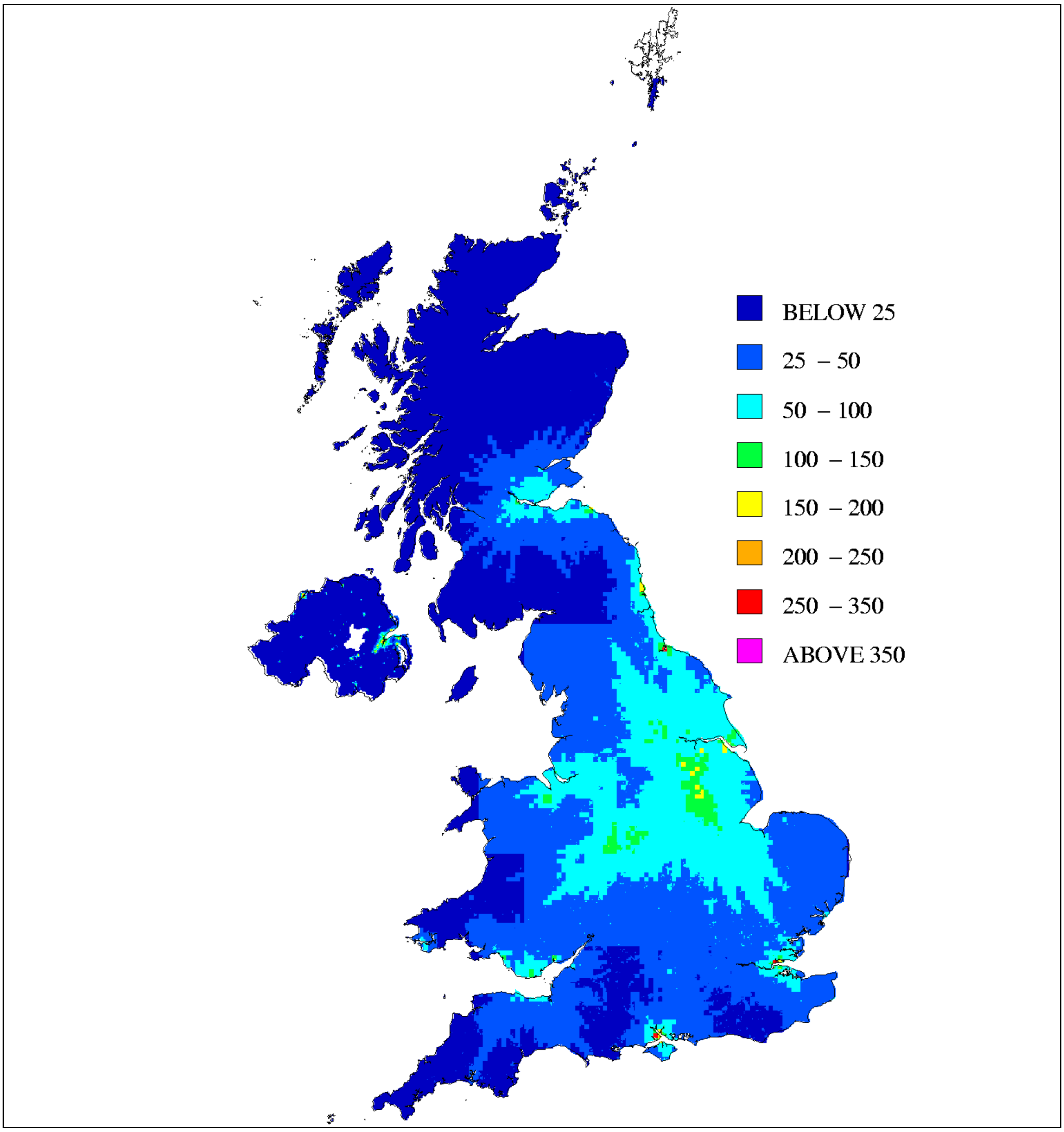


Figure 3.13: The 99.73th percentile of one-hour mean SO_2 concentrations 2002 ($\mu g\ m^{-3}$). Concentrations are predicted for 1 km x 1 km squares.

3.6 Method development

A number of potential improvements to the method would increase its utility in assessing the contribution of processes regulated by the Environment Agency to pollutant concentrations for the purposes of annual audit. These are:

- improved input data quality;
- increased modelling resolution;
- assessment of long-range effects of Environment Agency-regulated emissions on annual mean and winter mean concentrations;
- more consistent treatment of background concentrations;
- assessment of prediction intervals for modelled concentrations;

- spatial analysis of residual errors;
- preparation of incremental maps;
- site specific studies for areas where large pollutant concentrations are predicted or measured.

These developments are described in the following sections.

3.6.1 Improved input data quality

There are several areas where improved data quality might improve the performance of the models used for mapping pollutant concentrations:

- emissions;
- temporal variation in emissions;
- discharge characteristics;
- temporal variation in discharge characteristics;
- buildings effects;
- topography and surface roughness;
- meteorology.

The ADMS 3 dispersion model used by Netcen for mapping studies can take account of the available data on emissions and discharge characteristics and their temporal variation throughout the year. Obtaining high quality and reliable data on emissions and discharge characteristics would increase the credibility of model predictions and the Environment Agency should give high priority to improving the collection and collation of these data for regulated sources.

The ADMS 3 model can also take account of the effects of buildings close to discharge stacks on the dispersion of pollutants. Several buildings (up to 10) can be taken into account and the building most likely to affect dispersion can be allocated to each stack by the model user. The modelling study would benefit from information on the dimensions of buildings where these are likely to disturb dispersion from regulated sources.

ADMS 3 has the capacity to take account of spatial variations in terrain height and surface roughness and their effects on the wind field and dispersion. However, the spatial resolution of the complex terrain wind field model at the regional modelling scale is not sufficient to effectively distinguish terrain features likely to affect maximum ground level concentrations.

Meteorological data suitable for dispersion modelling is available from several locations throughout the United Kingdom. In many cases, the nearest meteorological station is a substantial distance from emission sources and receptor locations. Netcen's mapping method has usually assumed that meteorological data from a single station in England applies over the whole of the UK. Appendix 4 provides an analysis of the spatial variability of meteorological data based on data from 11 meteorological stations in England and Wales for 1999. It is concluded that the use of a single meteorological station is adequate for the purposes of the preparation of annual maps.

3.6.2 Increased model resolution

Netcen modelled the contribution from large industrial point sources at receptors spaced at 5 km x 5 km intervals on a rectangular grid. Contributions at intermediate points were then interpolated onto a 1 km x 1 km grid and added to contributions from other sources. The large point sources were modelled at the five km resolution because of limitations in older versions of the ADMS dispersion model. Newer versions of the ADMS model allow increased resolution, where faster computers can perform the calculations reasonably quickly. It is feasible to increase the resolution to 2 km x 2 km without leading to unacceptable computing times and this will lead to improved model predictions close to major sources of emission.

3.6.3 Long-range effects on annual mean and winter mean concentrations

The Netcen methodology does not take account of the contribution to annual mean and winter mean concentrations from large sources regulated by the Environment Agency that are over (typically) 50 km from the receptor locations. Similarly, the Netcen method does not take account of area sources at distances greater than 15 km from the receptor. The Environment Agency needs to estimate the contribution from these sources to sulphur dioxide concentrations at more distant receptors for the purposes of annual audit.

Sulphur dioxide reacts in the atmosphere to form sulphate aerosols. The rate of reaction is relatively slow, generally with a time constant of the order of 100 hours, so that the removal of sulphur dioxide by chemical reaction is relatively unimportant over distances of 100 km or less. However, at longer distances the loss of sulphur dioxide by reaction may become significant. A number of models have been developed to take account of the loss by chemical reaction over long distances in predictions of acid deposition. Straight-line trajectory models such as HARM and TRACK have been used extensively in the UK to predict acid deposition.

For the purposes of this project, the acid deposition model TRACK was used to predict contributions to annual average sulphur dioxide concentrations from large point sources greater than 50 km from each receptor and from area sources greater than 30 km from the receptor. ADMS 3 was used to predict the contribution from these sources closer to the receptor. A small change was made to the TRACK model code to prevent double counting of the emissions within 50 km or 30 km of the receptor locations.

The TRACK model uses the Lagrangian trajectory approach, where species concentrations and depositions at receptors are the outcome of a windrose-weighted sum of contributions from straight-line trajectories incoming on regular points of the compass. The original TRACK model assumed that each trajectory had a fixed cross-wind width, centred on the midpoint of each wind direction sector. This approach led to a ‘star pattern’ of predicted concentrations around large point sources. A small change was made to the TRACK model code so that emissions from across the whole of each wind direction sector would be taken into account (Appendix 8).

Earlier work for the Environment Agency had indicated that the TRACK model overestimated sulphur dioxide concentrations in remote areas of the UK (Abbott, 2003). Model input parameters were therefore reviewed. The NEGTAP report recognised that dry deposition velocities for sulphur dioxide increased as sulphur dioxide concentrations decreased. Measurements of sulphur dioxide dry deposition show that the affinity of absorbing surfaces for sulphur dioxide is strongly influenced by the presence of surface water and the chemical composition of the surface water. The ratio of the concentrations of ammonia and sulphur dioxide at the leaf surface is particularly important. Appendix 9 sets out some theoretical justification for the dependence of the surface resistance on ammonia concentrations.

A ‘big leaf’ resistance analogy model was used to estimate the dry deposition velocity for sulphur dioxide. The big leaf model made use of an analogy between the resistance to mass transfer from the atmosphere and electrical resistances. Separate resistances were assigned to:

- the aerodynamic resistance through the turbulent surface boundary layer;
- the laminar boundary layer;
- the resistance through the stomata of plant leaves;
- the resistance to deposition to non-stomatal areas of the plant and to the ground surface.

Each of the resistance components was evaluated following the EMEP Unified model parameterisation (http://www.emep.int/index_model.html). It was assumed that on average neutral stability atmospheric conditions would occur. Upper and lower estimates of the stomatal conductance were used in the assessment to provide upper and lower estimates of the deposition velocity. According to a summary of recent observations provided to EMEP, reasonable values for the canopy resistance of SO_2 in areas of low and high NH, and wet and dry conditions, can be summarised as shown in Table 3.4

Table 3.4: Basis of non-stomatal resistance scheme for SO_2, s m^{-1}

	Dry surfaces	Wet surfaces
High NH_3	80	40
Low NH_3	180	100

EMEP interpolates between these values, on the basis of the acidity ratio ($a_{sn} = 0.6x[SO_2]/[NH_3]$). The low ammonia values are multiplied by factors of 1.0, 0.61 and 0.37 for a_{sn} ratios of 2.0, 1.5 and 1.0. Table 3.5 shows acidity ratios calculated from measured concentrations at rural monitoring sites in the UK. At each site, the acidity ratio was less than unity and thus outside the range of the EMEP interpolation. A non-stomatal resistance of 40 s m^{-1} was therefore used in this assessment, corresponding to the lower limit of EMEP range for predominantly wet surfaces.

Table 3.5: Acidity ratios at rural sites in the UK, 2000

Site	Sulphur dioxide concentration, μg S m^{-3}	Ammonia concentration, μg m^{-3}	Acidity ratio
Bush	1.18	0.53	0.71
Lough Navar	0.18	0.45	0.13
Eskdalemuir	0.29	0.32	0.29
Yarner Wood	0.41	0.5	0.26
Stoke Ferry	1.14	2.44	0.15
High Muffles	1.55	0.73	0.68
Strathvaich Dam	0.101	0.09	0.36

Table 3.6 summarises the parameters used to calculate dry deposition velocities for sulphur dioxide. For the purposes of modelling, the dry deposition for night-time conditions was set equal to the minimum deposition velocity; for daytime conditions, the deposition velocity was set to the mean of the maximum and minimum values.

The TRACK model assumes that pollutants are well mixed throughout the boundary layer. This is a reasonable assumption where dry deposition velocities are low. However, a concentration gradient develops throughout the surface stress layer for relatively high dry deposition velocities, so that concentrations near the ground are less than the boundary layer average. For a fully-developed concentration boundary layer, the concentration at a typical monitor height (typically 2 m above ground) is given by:

$$C_s = C_{av} \frac{r_{a2} + r_b + r_c}{r_a + r_b + r_c}$$

where:

C_s and C_{av} are the surface and boundary layer averaged concentrations respectively;
r_b is the resistance through the laminar layer;

r_c is the surface resistance;
r_a is the aerodynamic resistance through the whole surface stress layer;
r_{a2} is the aerodynamic resistance through the bottom 2 m of the surface stress layer;

Table 3.6 shows the ratio C_s/C_{av} for a range of terrain types. In practice, terrain types are not homogeneous so that any particular location may be surrounded by a range of terrain types. For the modelling, we therefore proposed to use an average ratio of 0.74 to represent all terrain conditions.

Table 3.6: C_s/C_{av} ratio for a range of terrain types

	Arable	**Grass**	**Permanent crops**	**Forest**	**Surface water**	**Urban**	**Other**
Surface roughness, m	0.2	0.02	0.3	1	0.001	1	0.1
Friction velocity, m s^{-1}	0.50	0.36	0.54	0.68	0.27	0.68	0.45
Aerodynamic resistance, s m^{-1}	29.9	57.3	26.0	16.0	106.2	16.0	37.2
Laminar layer resistance, s m^{-1}	10.0	13.8	9.3	7.3	18.8	7.3	11.1
Non-stomatal surface resistance, s m^{-1}	40	40	40	40	1	40	40
Maximum stomatal conductance, mmol m^{-2} projected leaf area s^{-1}	356	321	320	159	0	0	320
Minimum stomatal conductance, mmol m^{-2} projected leaf area s^{-1}	4	3	3	21	0	0	3
Leaf area index maximum	3.5	3.5	3.5	5	0	0	3.5
Leaf area index minimum	0	2	0	3.5	0	0	2
Maximum deposition velocity, mm s^{-1}	17.3	11.1	18.4	21.8	7.9	15.8	14.8
Minimum deposition velocity, mm s^{-1}	12.5	9.0	13.3	16.5	7.9	15.8	11.3
Average deposition velocity, mm s^{-1}	14.9	10.0	15.8	19.2	7.9	15.8	13.1
Surface correction factor, high stomatal conductance	0.77	0.77	0.77	0.78	0.72	0.79	0.77
Surface correction factor, low stomatal	0.68	0.72	0.68	0.71	0.72	0.79	0.70

	Arable	Grass	Permanent crops	Forest	Surface water	Urban	Other
conductance							

3.6.4 More consistent treatment of background concentrations

Netcen's methodology takes account of background concentrations when calculating high percentile concentrations in the region of Environment Agency-regulated sources, by adding a multiple of the estimated annual average background. This method is consistent with the recommendations given in earlier Netcen research for the Environment Agency. Further investigation of methods for adding background concentrations is currently under way. The methodology will be adapted to take account of recommendations resulting from this work.

3.6.5 Assessment of prediction intervals for modelled concentrations

The Netcen methodology provides calibration plots of the modelled contribution from large point sources against the measured values. A calibration factor is derived from the best fit through the plotted points. The scatter of points about the best fit line provides a measure of uncertainty in the predictions made by the model of the source contribution. A simple statistical analysis can then be used to derive an estimate of the interval either side of the model prediction within which a specified percentage (for example, 97.5 per cent) of measurements might be expected to lie. This is known as the prediction interval.

Based on the measured concentrations, Y_i, corresponding to the modelled concentrations, x_i, i = 1,2,…n, it is expected with 100(1-a) percent confidence that the (unknown) measured concentration for a modelled concentration x_0 will be contained in the interval:

$$A + Bx_0 \pm t_{a/2,n-2}\sqrt{\left[\frac{(n+1)}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}}\right]\frac{SS_R}{(n-2)}}$$

where:

A and B are the least squares estimates of the intercept and slope;
$t_{a/2,\ n-2}$ is the Students t with confidence level a/2 and n-2 degrees of freedom;
S_{xx} is the sum of the squares of x-x_i;
SS_R is the sum of the squares of the residuals (Y_i-A-Bx_i).

For the case where the best-fit line is constrained to go through the origin, the interval is estimated by:

$$Bx_0 \pm t_{a/2,n-1}x_0\sqrt{\frac{SS_R}{S_{xx}(n-1)}}$$

Figure 3.14 shows the prediction interval (a = five per cent, n = 33) for the 99.73th percentile hourly sulphur dioxide concentration for 2003. Based on this analysis, it is estimated that there is less than 2.5 per cent chance that the concentration at a particular place is more than the objective of 350 μg m^{-3} if the calibrated model prediction is less than 265 μg m^{-3}.

The calculation of prediction intervals is thus straightforward and allows the risk of exceedence of the objectives to be assessed.

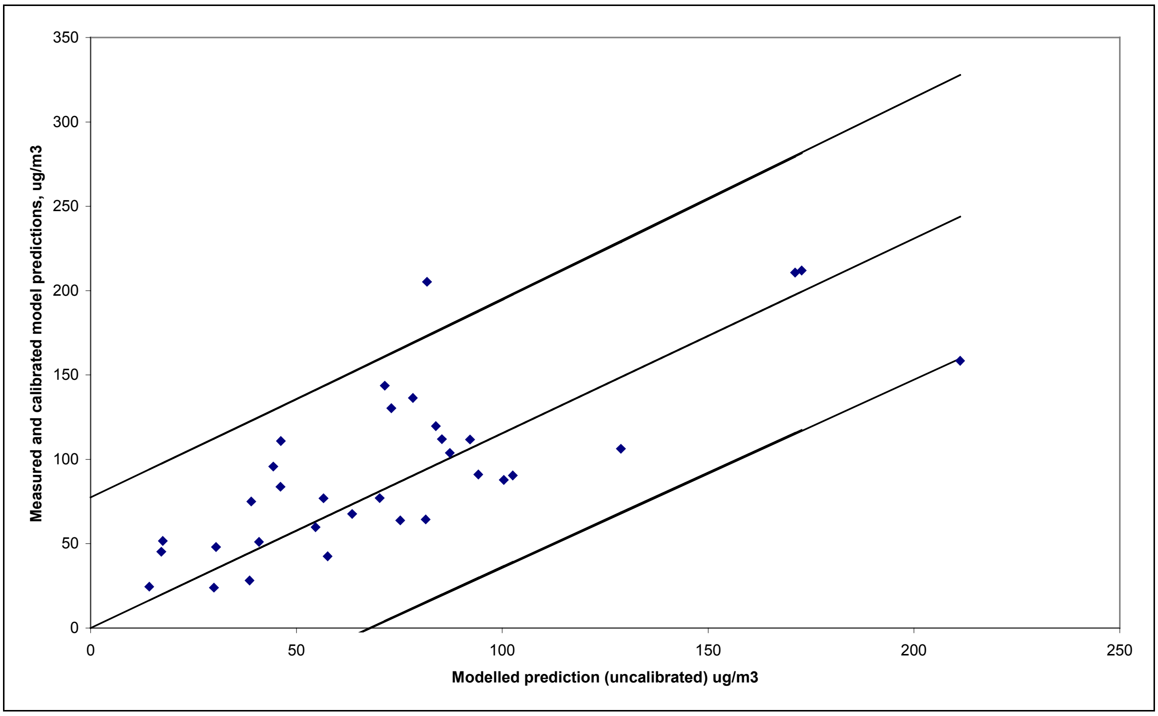


Figure 3.14: The prediction interval for the 99.73th percentile hourly sulphur dioxide concentration for 2003

3.6.6 Spatial analysis of residual errors

The dispersion modelling carried out by Netcen provides detailed maps of the concentrations of sulphur dioxide throughout the UK. Similar maps could also be generated simply by interpolation of measured concentrations. It is worthwhile considering whether the modelled maps provide improved estimates of pollutant concentrations.

A simple spatial analysis may be carried out as follows. If there are n monitoring stations, then there are n(n-1)/2 pairs of monitoring stations. For each pair of monitoring stations, calculate the variance of the measured concentrations and the distance between the monitoring stations. Order the pairs of monitoring stations in increasing order of distance. Then group the pairs by distance and calculate pooled estimates of variance for each distance range. The pooled variance estimates may then be plotted against distance between monitoring stations (the variogram).

Figure 3.15 shows the pooled variance of annual mean sulphur dioxide concentrations of pairs of monitoring stations plotted in this way. The pooled variance increases with increasing distance between the monitoring stations, while the concentrations measured at stations near to each other have less variance. The pooled variance estimates do not decrease monotonically to zero: extrapolation of the points to zero distance suggests that there is a finite intercept (the nugget) which may reflect localised variations in pollutant concentrations or measurement errors.

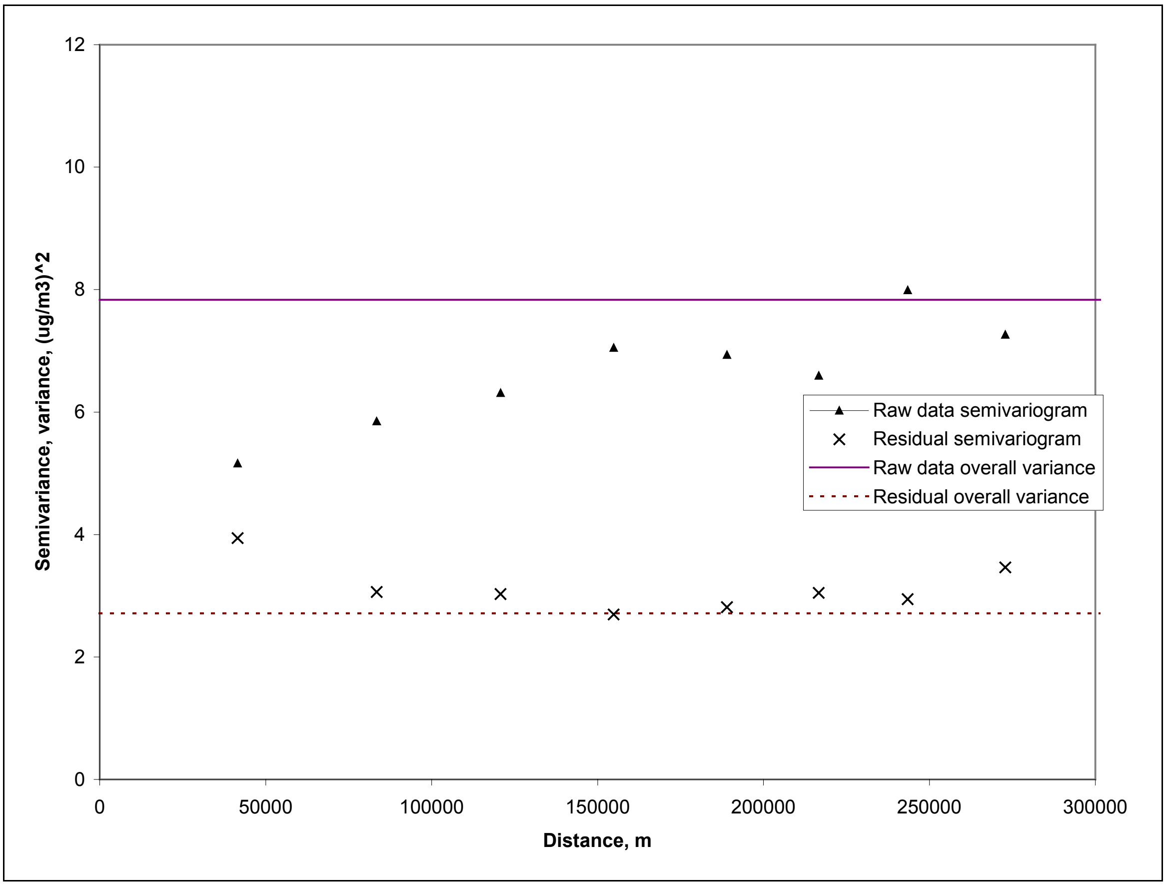


Figure 3.15: Spatial analysis of residuals: semi-variograms of monitoring data and model residuals for annual average SO_2

The difference between the modelled and measured concentrations at each monitoring station (the residuals) may be calculated and a similar variogram plotted. This variogram is also shown in Figure 3.15. The pooled variance of the residuals is markedly less than the pooled variance of the measured data, which indicates that much of the variance in the measured data has been explained by the model. The variance of the residual is greatest at short distances between monitoring stations: this feature is related to the spatial resolution of the model (5 km x 5 km). At distances of around 50 km and less, the variance of the residuals is similar to the variance of the measured data and it is suggested that the modelled maps would not provide much improvement over interpolated maps if monitoring stations were less than 50 km apart. In practice, monitoring stations are often rather more widely spaced. However, the analysis suggests that there is some deterioration in model performance in predicting annual mean concentrations at short distances. The deterioration may arise for a number of reasons: it is suggested that the most likely reasons relate to the model resolution or to errors in the emissions inventory.

3.6.7 Sensitivity studies

The selection of dispersion model input parameters requires an element of subjective judgement. For example, the model user selects a value of the surface roughness on the basis of an assessment of the terrain or land use. Weather data may be obtained from meteorological stations some distance from the receptor area. Consequently, there is some uncertainty in the model input data. Sensitivity studies may be carried out to assess the uncertainty in predicted pollutant concentrations resulting from the uncertainty in model inputs.

A Monte Carlo simulation based on an ADMS dispersion model of the emissions from Drax, Eggborough and Ferrybridge power stations was carried out in which the surface roughness was allowed to take values at random within the range 0-0.3 m. The uncertainty in the meteorological data was assessed (see Appendix 4). The wind direction for each hour of the year was selected from a normal distribution with standard deviation 20^{o} about the direction specified in the meteorological data. The wind speed was similarly selected from a normal distribution with standard deviation 0.75 m s^{-1} about the nominal value contained in the meteorological data, subject to an overriding minimum of 0.75 m s^{-1}. The cloud cover for each hour was selected from a normal distribution with standard deviation of one octa about the nominal value in the meteorological data within the range zero to eight octas. One hundred model runs were carried out.

Figure 3.16 shows a cumulative probability distribution of the predicted annual mean concentrations at a receptor at (448700, 426800) approximately two km north east of Ferrybridge power station. Figure 3.17 shows a similar plot of the cumulative probability of the 99.9th percentile 15-minute mean concentration. The analysis suggests that the annual average concentration in particular is sensitive to uncertainties in the input parameters.

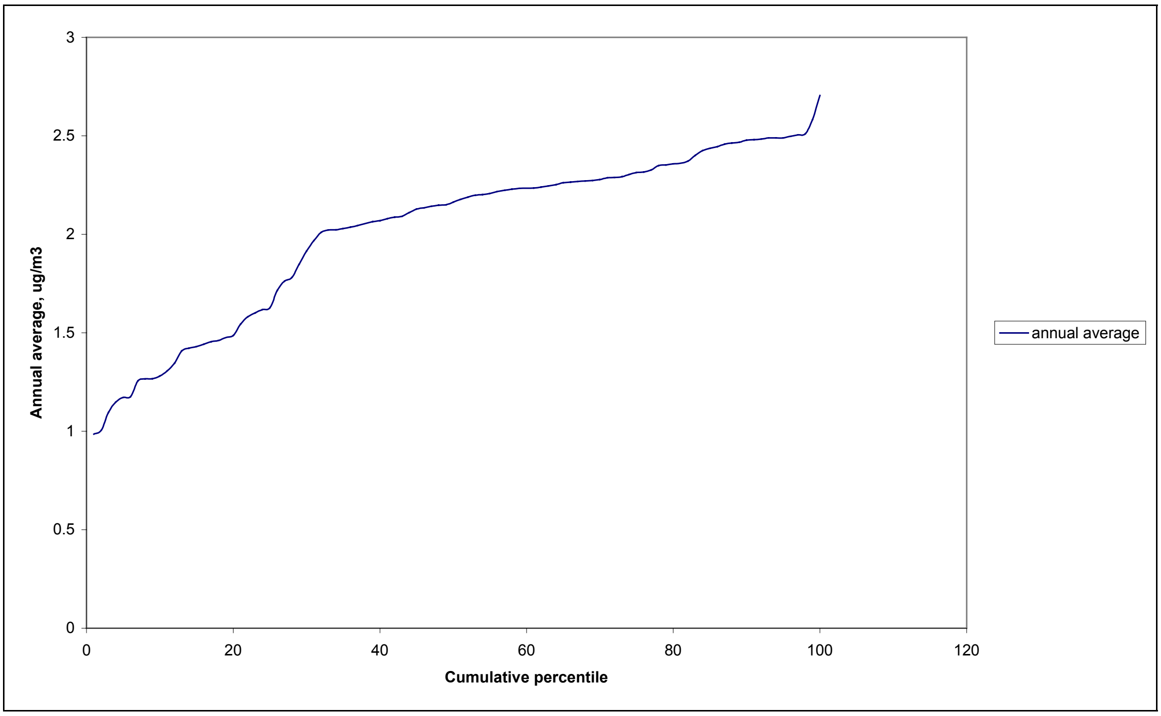


Figure 3.16: A cumulative probability distribution of the predicted annual mean concentration at a receptor approximately two km north east of Ferrybridge power station

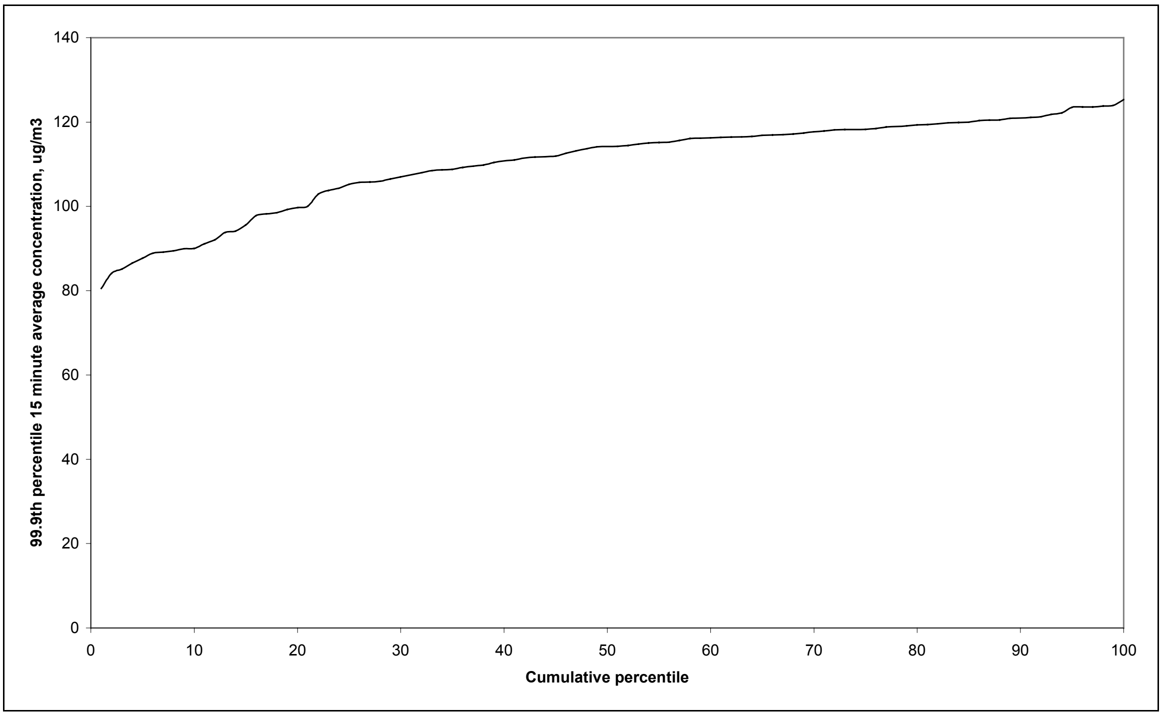


Figure 3.17: A cumulative probability distribution of the predicted 99.9th percentile 15 minute-mean concentration at a receptor approximately two km north east of Ferrybridge Power Station

3.6.8 Preparation of incremental maps

Two main aims of the annual audit are to:

- quantify the contribution to pollutant concentrations made by Environment Agency-regulated sources;
- identify which source sectors make the greatest contribution to pollutant concentrations.

The Netcen methodology for sulphur dioxide explicitly takes account of the contribution from the largest Environment Agency-regulated sources. For short-term objectives, it is illustrative to compare the contribution from Environment Agency-regulated sources or individual source sectors alone with the contribution from all sources; the regulated sources make the largest contribution to short-term peak concentrations over much of England and Wales, and contributions from individual source sectors mean the short-term concentrations cannot simply be added to provide an overall estimate of concentration.

For long-term objectives, contributions from individual source sectors may be added to provide the total concentration of sulphur dioxide. It is illustrative to compare the total concentration with and without Environment Agency-regulated sources or source sectors and to compare the contributions from individual source sectors.

The Netcen methodology is readily adapted to incorporate the contribution from Environment Agency-regulated sources in this way.

3.6.9 Site-specific studies for areas where large pollutant concentrations are predicted or measured

Pollutant concentration maps prepared by national modelling and mapping can identify those areas at greatest risk of exceeding air quality objectives. However, the methods make a number of assumptions that may not be applicable close to individual sources. More detailed modelling studies are appropriate where:

- modelled concentrations approach the air quality objectives, taking account of the uncertainty in the modelling approach and derived prediction intervals;
- measured concentrations at monitoring stations are larger than the modelled concentrations and are outside the expected prediction interval.

Detailed local modelling studies can take account of:

- more detailed emissions data, particularly temporal variation in emissions throughout the year;
- more detailed information of discharge arrangements - temperature and discharge velocities and their variation throughout the year;
- building dimensions;
- topography;
- meteorological data;
- monitoring data;
- increased model spatial resolution.

The ADMS3 model used for dispersion modelling in the preparation of Netcen maps can be readily applied to local modelling studies when detailed data on the local situation are available.

4 Netcen method for oxides of nitrogen

Netcen prepared national scale maps of nitrogen oxide concentrations for comparison with the air quality objectives and limit values presented in Table 4.1

Table 4.1: Air quality limit values and objectives for oxides of nitrogen

Pollutant	Air quality objective or limit value		Date to be achieved by
Nitrogen dioxide objective	40 $\mu g/m^3$	annual mean	31.12.2005
Nitrogen dioxide limit value Annual limit value for the protection of human health	40 $\mu g/m^3$	annual mean	1.1.2010
Oxides of nitrogen limit value Annual limit value for the protection of vegetation	30 $\mu g/m^3$	annual mean	19.7.2001

No attempt was made to model hourly concentrations for comparison with the one-hour limit value for nitrogen dioxide, because the annual mean limit value was expected to be more stringent than the one-hour limit value in the majority of situations (AQEG, 2003).

Special techniques have been developed to provide mapped estimates of roadside concentrations near to major roads throughout the United Kingdom.

4.1 Emission estimates and discharge conditions

All Part A processes within the National Atmospheric Emission Inventory with emissions greater than 500 tonnes per annum were included in the detailed dispersion modelling.

Prior to the modelling exercise, a survey of Part A authorisation notices held by the Environment Agency was conducted for all point sources with annual emissions greater than 500 tonnes, as identified in the 2001 NAEI. Parameters characterising the release to atmosphere were collected; these were:

- stack height
- stack diameter
- discharge velocity
- discharge temperature.

Where release parameters were unavailable, engineering assumptions were applied. Previously collated data sets on emission release parameters from large SO_2 point sources were also used to characterise the release of emissions (Abbott and Vincent, 1999).

Many of the Part A processes emit oxides of nitrogen through multiple stacks. We have ignored the possible enhancement of plume rise that may occur when plumes combine from stacks located near to each other. Where there are many stacks at the same site with different discharge conditions, for example at refineries or chemical works, we have, in some cases, grouped stacks of similar height and discharge characteristics together and assumed that the emission from each group of stacks may be represented by a single stack with characteristics of the stack with the largest emission or by a stack with an emission-weighted ‘average’ stack.

Appendix 5 lists the emission rates and discharge characteristics used for modelling 2003 oxides of nitrogen emissions.

Power stations do not produce electricity at a constant rate, with electricity generation increasing and decreasing with demand. However, a constant emission rate was assumed for the purposes of modelling annual average oxides of nitrogen concentrations.

Emissions from smaller industrial sources regulated by the Environment Agency with emissions of less than 500 tonnes per annum were obtained from the NAEI on a 1 km x 1 km basis. The NAEI provides no details of the discharge conditions from these smaller industrial sources of emissions of nitrogen oxides. It was therefore assumed that the discharge height met the requirements of the Chimney Heights Memorandum, 3rd edition. Other assumptions included a discharge temperature of 100°C, a discharge velocity of 10 m s^{-1}, an emission factor of 0.1 g MJ^{-1} and oxides of nitrogen concentrations in the discharge of 300 mg m^{-3} at reference conditions. Further details are given in Appendix 2.

Estimates of emissions from domestic, transport, Part B industrial sources and other area sources were obtained from the NAEI for each three km square area. The emissions from each road transport source were assumed to be distributed uniformly through an initial height of 10 m, where each three km source was represented by an emitting volume 3 km x 3 km square and 10 m high. The estimate of 10 m is based on the height of a typical house and assumes that road transport emissions will be entrained in the wake of nearby buildings. For other area sources, it was assumed that the initial emitting volume was 30 m high, corresponding to buoyant emissions from discharge stacks at small industrial or institutional premises. For road transport, it was assumed that the emissions varied throughout the week according to a profile obtained from an analysis of the distribution of all traffic in the United Kingdom by time of day (Road Traffic Statistics, 1999, Department of Transport) (Figure 4.1). A constant rate of emission was assumed for other area sources.

National Atmospheric Emission Inventory estimates of aircraft emissions include emissions throughout the whole of the take-off and landing cycle. Only a small part of the emission is released near ground level and contributes to ground level oxides of nitrogen concentrations. A factor of 0.36 was applied to the aircraft emissions, representing that fraction emitted near to the ground. Similarly, a factor of 0.25 was applied to NAEI estimates of shipping emissions.

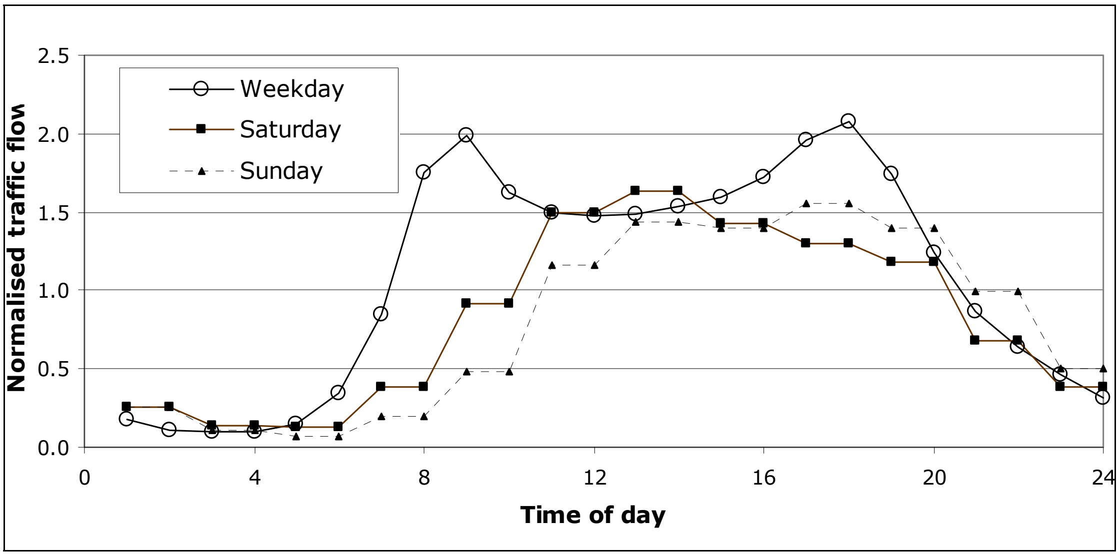


Figure 4.1: Temporal profile of traffic emissions

4.2 Dispersion modelling

Netcen used the dispersion model, ADMS Version 3.1, to calculate oxides of nitrogen concentrations. The contributions from large industrial sources, small industrial sources and other area sources were modelled separately: methods used are described below.

4.2.1 Large industrial sources

A receptor area was identified for each of the large industrial sources identified. The receptor areas cover an area of 100 km x 100 km centred on the midpoint of the 1 km x 1 km OS grid square containing the industrial source. The receptors were spaced on a rectangular grid at five km intervals over the receptor area.

Various data sets have been used to represent meteorological conditions. Most recently, sequential hourly data from Waddington for 2002 and 2003 obtained from the Meteorological Office has been used to represent meteorological conditions throughout the whole country for the appropriate year for the purposes of modelling the contribution from large Part A processes. The sequential data provides hourly information of windspeed, wind direction, cloud cover, relative humidity and precipitation. A uniform surface roughness of 0.1 m, typical of agricultural areas was used for the whole country. The effects of buildings and complex terrain have not been taken into account.

4.2.2 Area sources

The annual average contribution from area sources other than small Part A industrial sources was calculated on a one km receptor grid covering the country using the dispersion model ADMS Version 3.1. A dispersion kernel approach as described in 3.2.2 was used. Separate dispersion kernels were prepared for traffic emissions and for domestic and other emissions. Table 4.2 shows the dispersion parameters used to calculate the dispersion kernels. Dispersion kernels based on gridded emission sources at one km, three km and five km intervals have variously been used. The most recent maps have used kernels based on three km gridded emission sources. Hourly sequential meteorological data for Heathrow for the years 1993-2002 was used to prepare the dispersion kernels.

Table 4.2: Dispersion parameters used to calculate area source kernels

	Traffic kernel	**Constant kernel**
Surface roughness	1 m	1 m
Emission factors	Varying (see below)	Constant
Height of well-mixed source	10 m	30 m
Hourly sequential meteorological data	Yes	Yes
Minimum Monin-Obukhov length	30 m	30 m
Emission from each volume source	1 g s^{-1}	1 g s^{-1}
Number of receptor grids (model extent):		
One km area source model	31 (31 km)	31 (31 km)
Three km area source model	11 (33 km)	11 (33 km)
Five km area source model	7 (35 km)	7 (35 km)

A similar approach was used for small industrial sources regulated by the Environment Agency. However, a non-linear correction factor was used to take account of stack height, plume momentum and buoyancy effects from point sources:

$$c_{l,m} = \sum_{i=-15}^{15} \sum_{j=-15}^{15} k_{i,j} 20 \left(\frac{e_{l+i,m+j}}{20} \right)^{0.6}$$

An in-square contribution from small point sources was also calculated, because the point source is unlikely to be located at the centre of the grid square:

$$C = 1.54\log_{10}(10q)+0.464$$

where C is the in-square concentration, μg m^{-3}; q is the emission rate, g s^{-1}; and 1.54 is a numerical constant, calculated as the average value over the years 1993-2002 for meteorological data at Heathrow

The derivation of these empirical adjustments is given in Appendix 2.

4.3 Contribution from rural background concentrations

Diffusion tube measurement data from the acid deposition monitoring network were used to estimate rural annual mean background NO_x concentrations. Rural NO_x concentrations were derived from the NO_2 concentrations measured by the diffusion tubes by multiplying the rural NO_2 concentration by a factor of 1.28, derived from empirical analysis of monitoring data from continuous monitoring sites. In a number of instances, measurements from this network were influenced by contributions from nearby point and area sources. Contributions from point and area sources, estimated by dispersion modelling, were subtracted from the rural background measurement data to avoid double counting of these contributions. The correction procedure is as follows:

Corrected rural background (μg m^{-3}) = uncorrected rural background (μg m^{-3}) – (kA + B + C)

where A = modelled contribution from area source components;
k = empirical coefficient derived from a comparison of the previous year's monitoring data and model outputs (nominally k = 1);

B = sum of modelled contributions from large point sources;
C = sum of modelled contributions from small point sources.

Corrected rural measurement data were interpolated to obtain estimates of the regional background concentration throughout the UK.

4.4 Area source model calibration

The modelled oxides of nitrogen concentrations were then compared with oxides of nitrogen concentrations obtained at rural, suburban, urban background and urban centre monitoring sites in Defra's Automatic and Urban Rural Network. The modelled contributions from large and small point sources and the interpolated corrected rural background concentrations were subtracted from the measured concentrations: the remainder was then compared with the modelled contribution from area sources. Figure 4.2 shows this remainder plotted against the modelled prediction of the area source contribution. Examination of Figure 4.2 shows that the monitoring sites fall into two groups:

- inner conurbations
- elsewhere.

'Inner conurbations' include inner and central London and central Birmingham and Manchester, as defined by the Department for Transport (DfT, 2003). The 'elsewhere' slope is close to unity, showing that in these locations the uncalibrated model is quite successful in predicting the concentration. The inner conurbations slope is lower and reflects the different meteorological and dispersion conditions in the centres of larger cites. Meteorological data from Heathrow is not expected to be representative of central London, for example. The effective roughness in large urban areas is also greater than in rural or smaller urban areas, leading to more efficient dispersion of pollutants. Urban heat island effects in large cities limit the frequency of stable atmospheric conditions that contribute to elevated oxides of nitrogen concentrations elsewhere.

The selection of the empirical coefficient, k, in Section 4.3 above is in principle an iterative process. However, in practice, one iteration is usually sufficient.

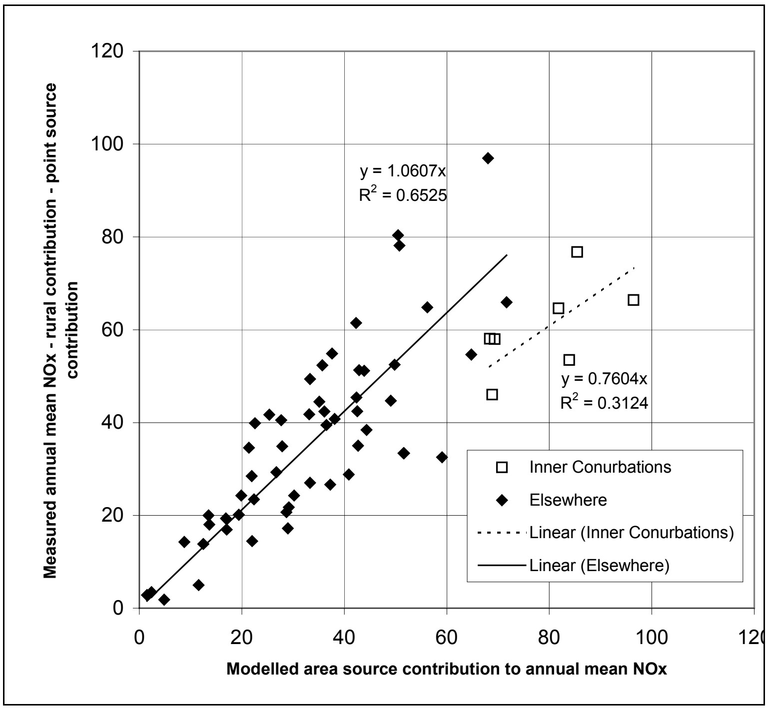


Figure 4.2: Calibration of NO_x area source model

4.5 Addition of modelled contributions to the corrected rural background concentration

Total annual average NO_x concentrations are calculated as the sum of:

- the modelled large point source contributions;
- the modelled small point source contributions;
- the corrected rural background concentration;
- the calibrated modelled area source contribution.

4.6 Conversion of oxides of nitrogen to nitrogen dioxide

Various empirical relationships have been used by Netcen to predict annual average nitrogen dioxide concentrations from the modelled oxides of nitrogen concentrations at background (non-roadside) locations. The most recent report describes the maps prepared for 2002, in which the following relationships were used:

Rural background NO_2 ($\mu g/m^3$) = *$0.7835NO_x$ ($\mu g/m^3$, as NO_2)*
Central London background NO_2 ($\mu g/m^3$) = *$2.28(NO_x (\mu g/m^3, \text{as } NO_2))^{0.6887}$*
Inner London background NO_2 ($\mu g/m^3$) = *$2.16(NO_x (\mu g/m^3, \text{as } NO_2))^{0.6887}$*
Outer London background NO_2 ($\mu g/m^3$) = *$2.04(NO_x (\mu g/m^3, \text{as } NO_2))^{0.6887}$*
Elsewhere urban background NO_2 ($\mu g/m^3$) = *$1.9301(NO_x (\mu g/m^3, \text{as } NO_2))^{0.6887}$*

The relationship for rural background concentrations was derived from monitoring data from 1998 to 2001 inclusively. The relationships for urban areas were derived from monitoring data from 1998 to 2002 inclusively and are presented in Figure 4.3. The relationships reflect the contrast between the behaviour of NO_x, which can be treated as a conserved pollutant, and NO_2, for which the ambient concentration is dependent on the availability of oxidant and the distance from source. The majority of NO_x is present as NO_2 at rural background locations because such areas are generally distant from sources and oxidant (ozone) is available in excess. Annual mean NO_2 concentrations in urban areas (Figure 4.3) are, however, limited by the availability of oxidant. From Figure 4.3 it is can also been seen that measured NO_2 concentrations at the same measured NO_x concentration increase from ‘elsewhere’ through outer and inner to central London. This is thought to be due to the large size of the Greater London urban area, which enables relatively aged NO_x from other parts of London to contribute to NO_2 in central London. We have used the definitions of outer, inner and central London adopted within the DfT transport models (DfT, 2003).

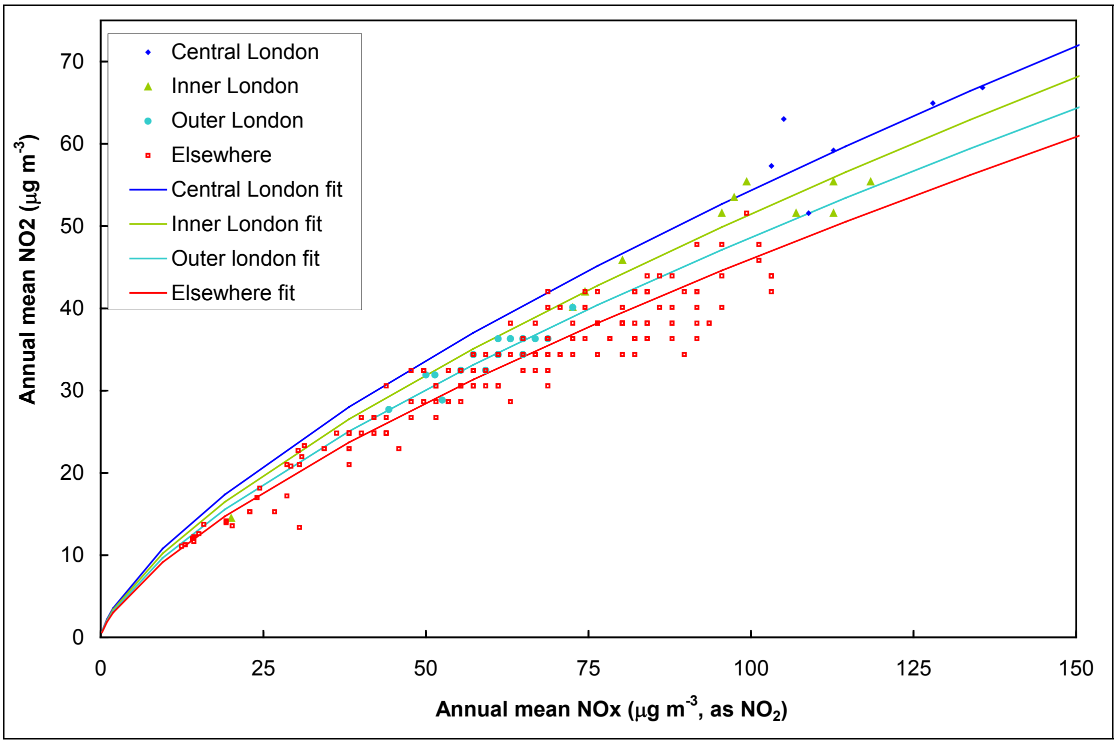


Figure 4.3: Relationship between annual mean NO_x and NO_2 concentrations measured at urban background sites in the national networks 1998-2002

More recently, the conversion of oxides of nitrogen to nitrogen dioxide has been considered by Defra’s Air Quality Expert Group (AQEG). The analysis represented in the AQEG report suggested that total oxidant (ozone plus nitrogen dioxide) concentrations are related to oxides of nitrogen concentrations by the relationship of the form:

$$[OX] = A[NO_x] + B$$

where B is the regional OX concentration, B = 35.7 ppb, and A is related to the proportion of NO_x emitted from the source as nitrogen dioxide (best fit to data A = 0.0948).

$[NO_2]/[OX]$ ratios are then obtained as a function of $[NO_x]$ concentrations as polynomial fits to monitoring data.

Fit 1 is applied at background sites in London:

$$[NO_2]/[OX] = (1.015 \times 10^{-1}) + (1.367 \times 10^{-2} [NO_x]) – (6.127 \times 10^{-5} [NO_x]^2) – (4.464 \times 10^{-8} [NO_x]^3)$$

Applicable range, 19 to172 µg m^{-3} NO_x as NO_2 (10 to 90 ppb).

Fit 2 is applied at sites near roads in London:

$[NO_2]/[OX] = (8.962 \times 10^{-2}) + (1.474 \times 10^{-2} [NO_x]) - (1.290 \times 10^{-4} [NO_x]^2) + (5.527 \times 10^{-7} [NO_x]^3) - (8.906 \times 10^{-10} [NO_x]^4)$

Applicable range, 19 to 402 µg m^{-3} NO_x as NO_2 (10 to 210 ppb).

The Netcen maps currently under preparation for 2003 will use relationships of this type, although the polynomials used to represent the $[NO_2]/[OX]$ relationships may change.

Netcen's constant oxidant flux model was also used to calculate NOx/NO_2 ratios taking account of meteorology, mixing of ozone from the urban canopy and chemical kinetics. The model is based on a mass balance on vertical elements within the surface boundary layer:

$$\frac{\partial}{\partial z}\left(\frac{ku^* z}{\phi}\frac{\partial[NO]}{\partial z}\right) - k_1[NO][O_3] + J[NO_2] = 0$$

$$\frac{\partial}{\partial z}\left(\frac{ku^* z}{\phi}\frac{\partial[O_3]}{\partial z}\right) - k_1[NO][O_3] + J[NO_2] = 0$$

$$\frac{\partial}{\partial z}\left(\frac{ku^* z}{\phi}\frac{\partial[NO_2]}{\partial z}\right) + k_1[NO][O_3] - J[NO_2] = 0$$

where:

k is the von Karman constant, equal to 0.4;
u^* is the friction velocity;
z is the height above the displacement height;
φ is a stability related factor;
k_1 is the rate of reaction between ozone and nitric oxide producing nitrogen dioxide;
J is the rate of photochemical reaction of nitrogen dioxide to form nitric oxide and ozone.

The upper boundary condition is at r = H/10, $[NO] = [NO]_{mbl}$, and so on.

The lower boundary condition is at z = 0:

$$\frac{ku^* z}{\phi}\frac{\partial[NO]}{\partial z} = -E_{NO} + v_d[NO]$$

where:

E_{NO} is the rate of emission of nitric oxide;
v_d is the non-aerodynamic deposition velocity, equal to $1/(r_b+r_{sur})$.

Boundary conditions applied take account of the proportion of oxides of nitrogen emitted as nitrogen dioxide (A) and the regional oxidant concentration (B). Figure 4.4 shows the predicted nitrogen dioxide concentrations as a function of oxides of nitrogen concentrations, evaluating the model for annual average parameters (k_1, J, u*) selected a priori. The model generates reasonable agreement with monitoring data from urban background sites throughout the UK. In practice, the predictions are little different from the AQEG polynomial fit (Jenkin's Fit 1)

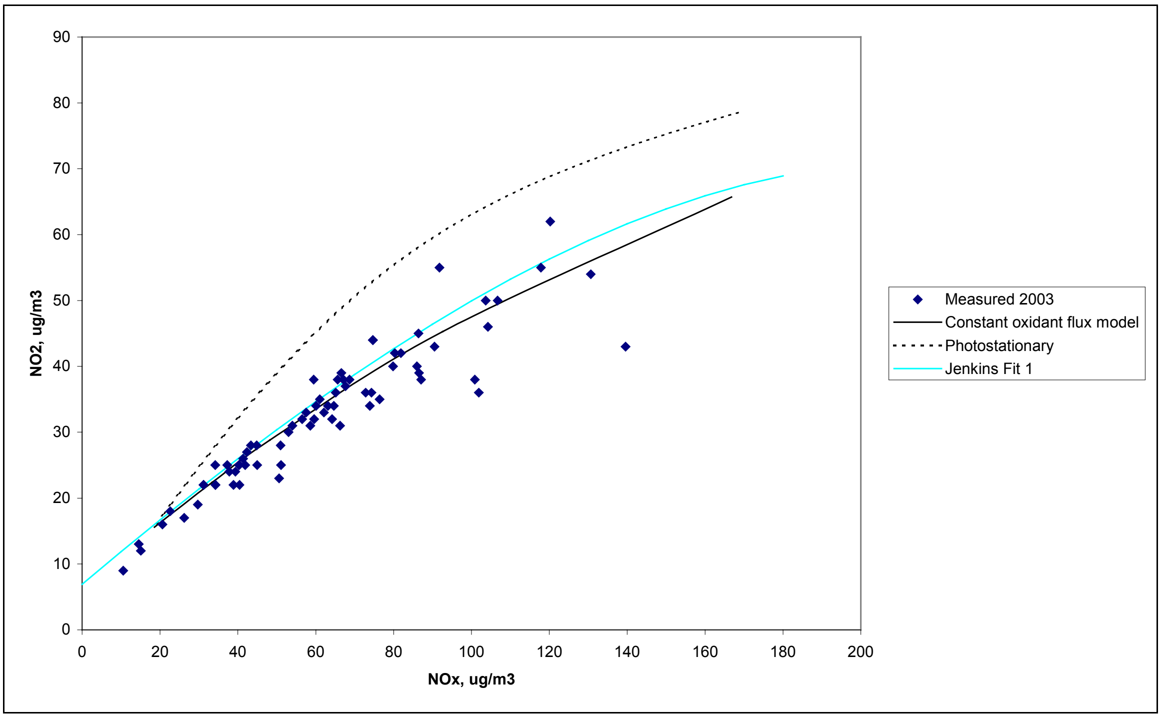


Figure 4.4: A comparison of measured NO_2 concentrations and a number of methods used to predict NO_2 concentrations

The AQEG empirical relationships apply where oxides of nitrogen are emitted at ground level. Large point sources on the other hand generally release oxides of nitrogen above the constant flux surface boundary layer, so that the empirical relationship may not apply. Figure 4.5 shows the corresponding plot of ground level NO_x and NO_2 concentrations for an elevated source. The constant oxidant flux predictions approach the photostationary state values, particularly at low oxides of nitrogen concentrations.

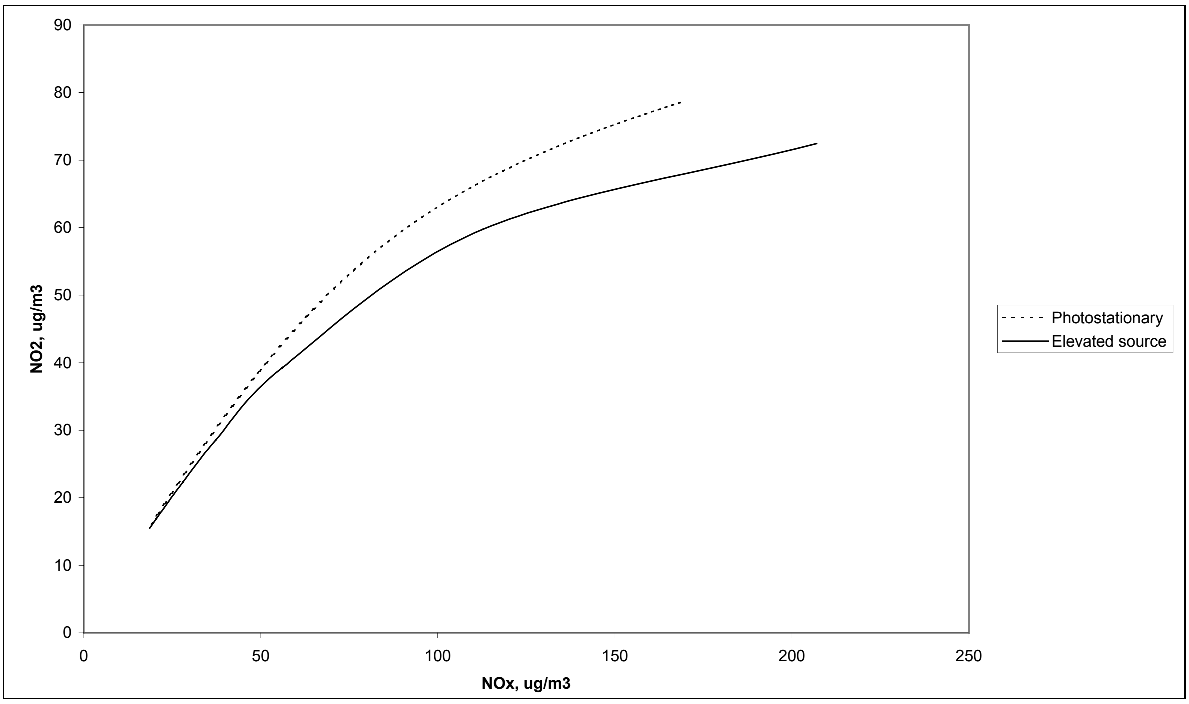


Figure 4.5: A comparison of two different methods to predict NO_2 concentrations following emission of NO_x from a large point source

4.7 Preparation of maps

Netcen currently prepare the required maps using the Geographical Information System ArcInfo, which was used here. Simple scripts were prepared in the ArcInfo command language (*.aml) to facilitate the data handling operations.

Figure 4.6 shows the Netcen map prepared for nitrogen dioxide concentrations for 2002. Figure 4.7 similarly shows the Netcen map for annual average oxides of nitrogen concentrations for 2002, which is relevant to the protection of vegetation (see Table 1.2). A data mask was applied in ArcInfo to exclude those areas where the annual average limit value for oxides of nitrogen did not apply.

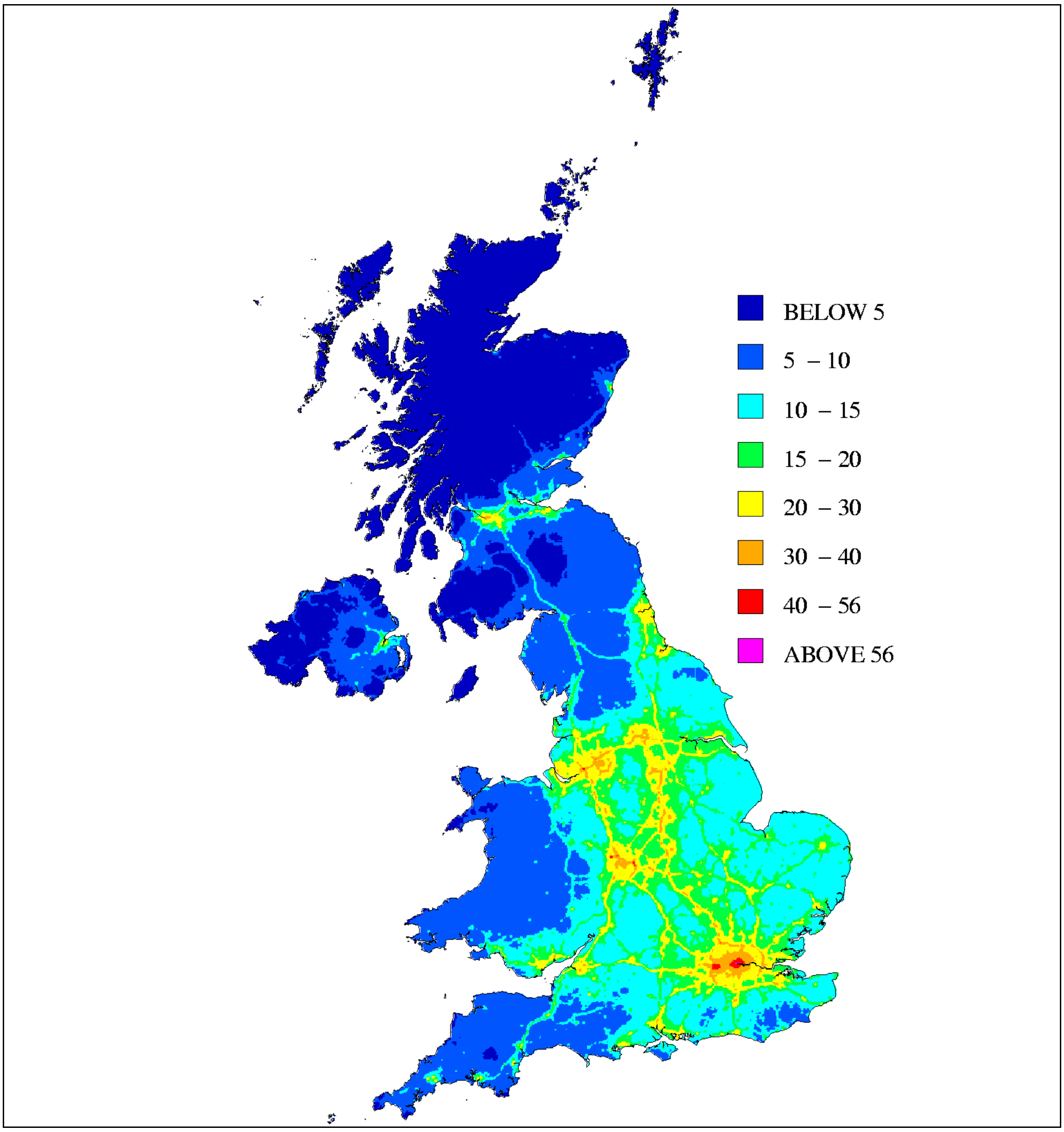


Figure 4.6: Annual mean background NO_2 concentration, 2002 ($\mu g\ m^{-3}$). Concentrations are predicted for 1 km x 1 km squares.

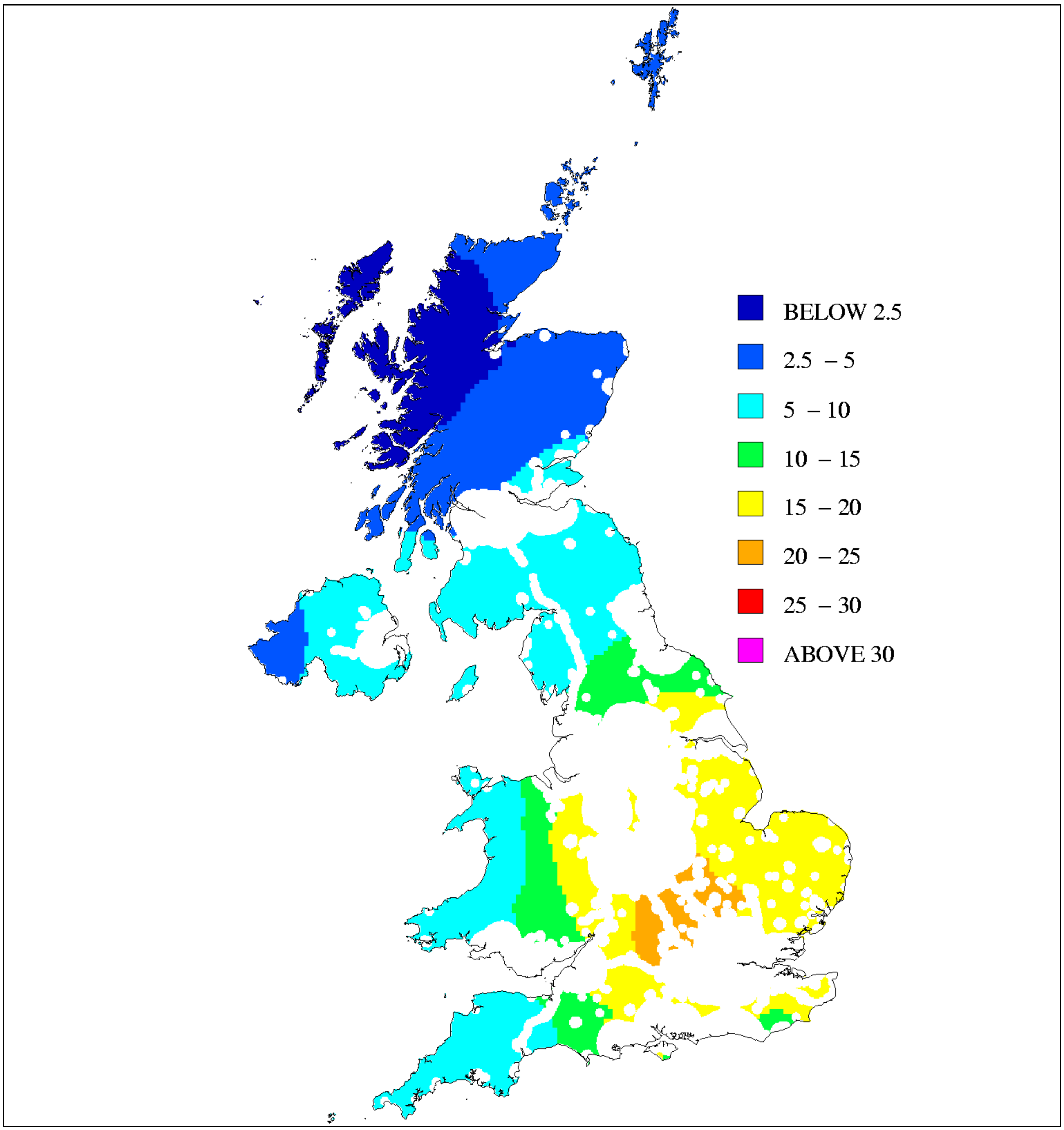


Figure 4.7: Annual mean rural NO_x concentration, 2002 ($\mu g\ m^{-3}$, as NO_2). Concentrations are predicted for 1 km x 1 km squares.

4.8 Roadside concentrations

Netcen also developed empirical techniques to estimate roadside oxides of nitrogen and nitrogen dioxide concentrations. The annual mean concentration of NO_x at a roadside location is made up of two parts: the background concentration (as described above) and a roadside increment:

Roadside NO_x concentration = background NO_x concentration + NO_x roadside increment

The roadside increment was estimated at roadside monitoring stations: the background NO_x component was derived from the map described above and subtracted from the measured roadside NO_x concentration.

The NAEI provides estimates of NO_x emissions for major road links in the UK. Netcen have assumed that the roadside increment is related to the emission per unit length of road, E, by means of a relationship of the form:

$$NOx\_roadside\_increment = kfE$$

where:

k is an empirical constant for oxides of nitrogen, typically 0.18 s m^{-2};
f is an empirical adjustment factor that takes account of the annual average daily traffic flow and the type of road (Figure 4.8).

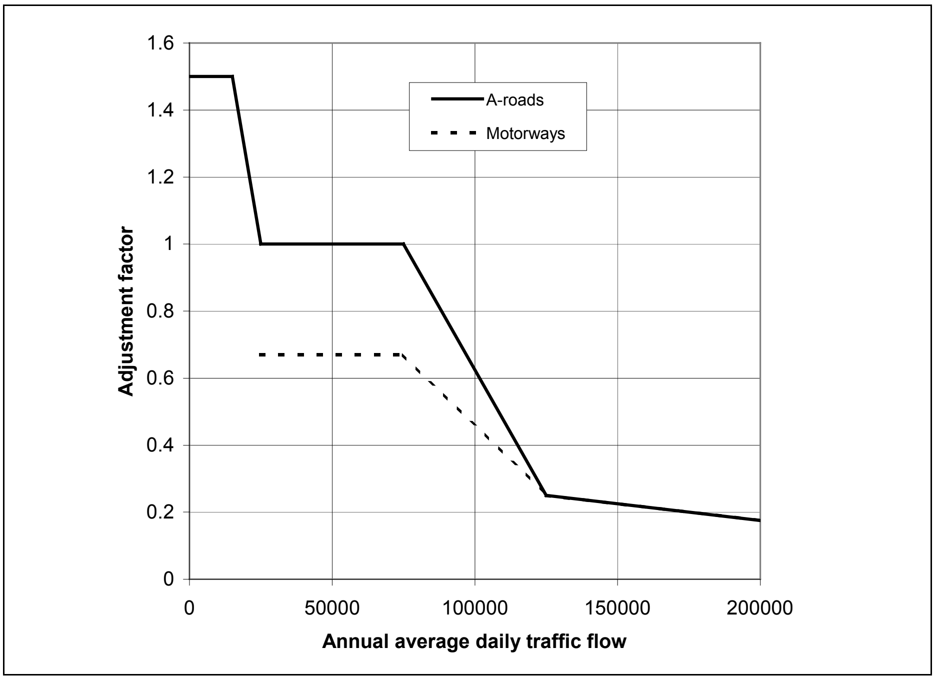


Figure 4.8: Adjustment factors applied to road link emissions

Netcen calculated nitrogen dioxide roadside increment for 2002 using the method developed by Laxen and Wilson (2002) included in the Highways Agency Design Manual for Roads and Bridges:

NO_2 roadside increment ($\mu g/m^3$) = NO_x roadside increment ($\mu g/m^3$, as NO_2) .
(0.53 - 0.068.ln(total roadside NO_x concentration ($\mu g/m^3$, as NO_2)))

Figure 4.9 shows the empirical map produced by Netcen of roadside nitrogen dioxide concentrations for 2002.

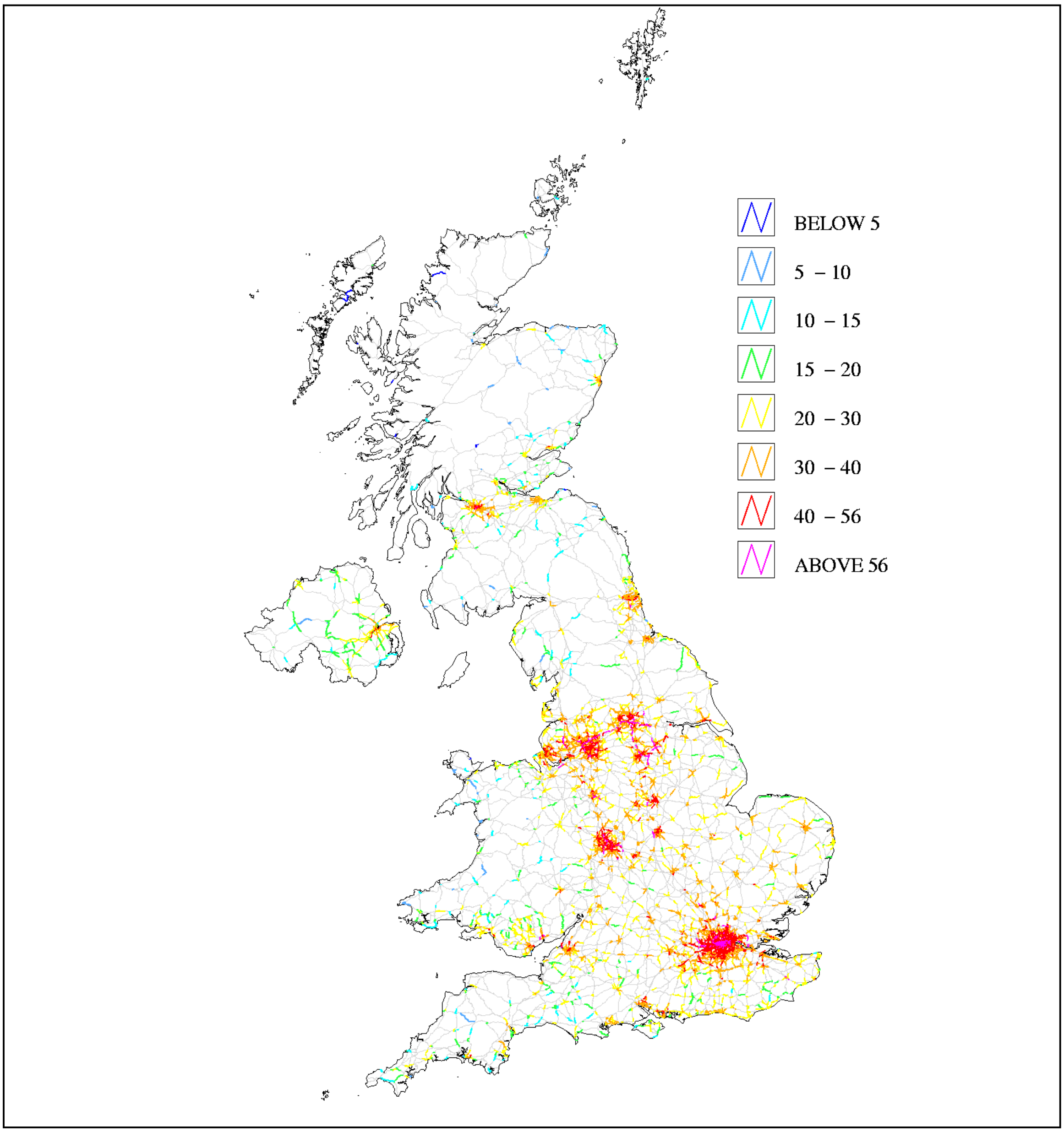
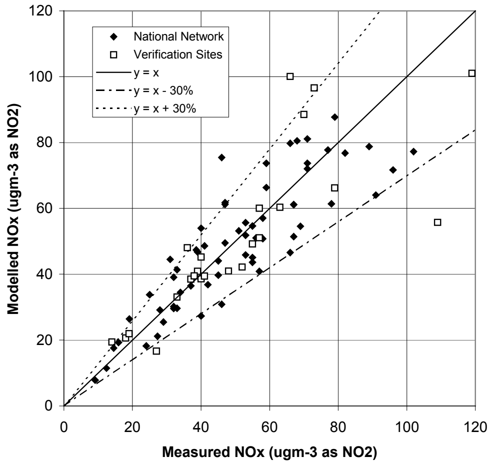


Figure 4.9: Major built-up roads, annual mean roadside NO_2 concentration, 2002 ($\mu g\ m^{-3}$)

4.9 Model verification

Modelled annual average oxides of nitrogen concentrations were compared with measured concentrations at monitoring sites throughout the UK. The sites used in the verification process included sites other than those in Defra's automatic urban and rural nnetworks. Data from sites quality assured by Netcen under contract but not part of the national network, including local authority sites in the Netcen Calibration Club, were therefore used for the verification of modelled estimates. The term 'verification sites' is used to describe all monitoring sites included in the verification analysis. Monitoring sites used for this comparison are listed in Appendix 6. Sites with a data capture of at least 50 per cent were included in the verification analysis. A higher data capture threshold of 75 per cent was applied for the national network sites used to calibrate the models.

Figure 4.10 to Figure 4.13 show verification plots of measured and modelled NO_x and NO_2 concentrations at background and roadside monitoring sites.



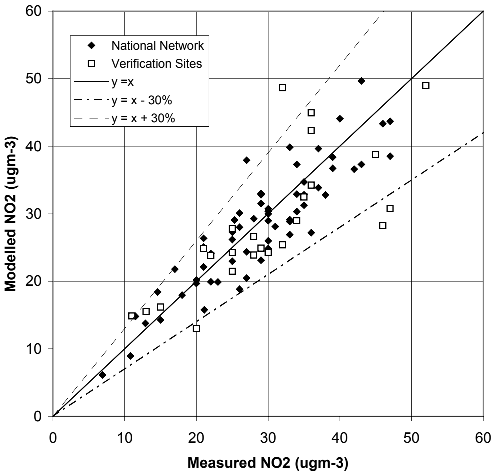
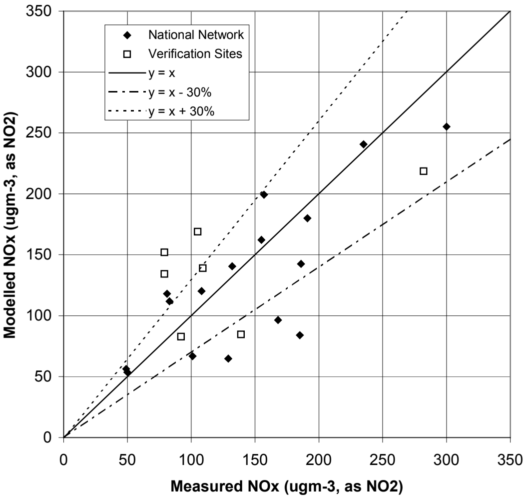


Figure 4.10 Verification of background annual mean NO_x model 2002

Figure 4.11 Verification of background annual mean NO_2 model 2002



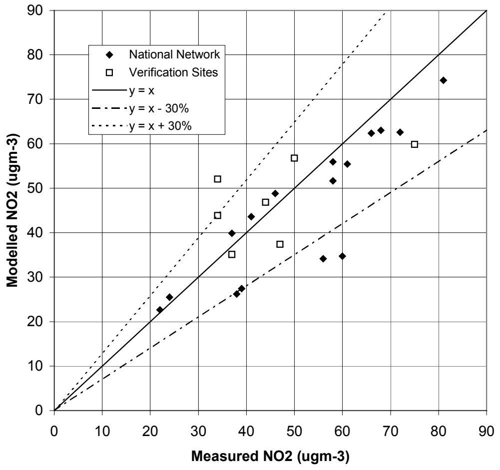


Figure 4.12 Verification of roadside annual mean NO_x model 2002

Figure 4.13 Verification of roadside annual mean NO_2 model 2002

4.10 Model development

A number of potential improvements to the method, similar to those for sulphur dioxide, would increase its utility in assessing the contribution of processes regulated by the Environment Agency to oxides of nitrogen concentrations for the purposes of annual audit. These include:

- calculation of high percentile nitrogen dioxide concentrations;
- improved methods of estimating NO_x to NO_2 conversion;
- improved input data quality;
- increased modelling resolution;
- assessment of long-range effects of Environment Agency-regulated emissions on annual mean concentrations;
- more consistent treatment of background concentrations;
- assessment of prediction intervals for modelled concentrations;
- spatial analysis of residual errors;
- preparation of incremental maps;

- site-specific studies for areas where large pollutant concentrations are predicted or measured.

Specific improvements relating to oxides of nitrogen modelling are described in the following sections.

4.10.1 High percentile nitrogen dioxide concentrations

Netcen have not prepared maps of the 99.8th percentile hourly average nitrogen dioxide concentration for comparison with the short-term objective or limit value because in most locations, the annual average objective is more stringent. However, the Environment Agency has a special interest in the regulation of large point sources, which may produce local exceedence of the short-term objective. Maps showing areas of potential exceedences of short-term objectives are therefore required by the Environment Agency.

The ADMS dispersion model can be used to produce maps of the 99.8th percentile of hourly mean oxides of nitrogen concentration in the same way as the 15-minute and hourly percentiles are prepared for sulphur dioxide. Nitric oxide, the main constituent of combustion emissions of oxides of nitrogen, reacts with ozone in the atmosphere to create nitrogen dioxide: the reverse reaction also occurs as the result of photodissociation of the nitrogen dioxide. The ADMS dispersion model used by Netcen includes a chemistry model that takes account of these reactions.

The ADMS chemistry module requires estimates of background ozone, nitrogen dioxide and nitric oxide concentrations for each hour. Cambridge Environmental Research Consultants (CERC), the model developers, recommend the use of monitoring data from the nearest rural background monitoring site in rural areas and the nearest urban background site for urban areas. The modelling studies for annual audit need to take account of all receptors in (typically) a 100 km square, and so some of the receptors will be in urban areas and some will be in rural areas. Most of the largest sources of emission are in rural areas. Therefore, the background monitoring site closest to the meteorological station should be used for the preparation of annual audit maps.

The ADMS chemistry module also requires an estimate of the proportion of oxides of nitrogen emitted as nitrogen dioxide. Typically, it has usually been assumed that 5-10 per cent of the oxides of nitrogen are emitted as nitrogen dioxide: however, there is little data supporting this assumption. Furthermore, the ADMS chemistry module does not take account of the reaction:

$$2NO+O_2 \rightarrow 2NO_2$$

which may be significant close to the point of discharge from the stack, where nitric oxide concentrations are relatively high. It is anticipated that analysis of data from monitoring sites near to power stations as part of the umbrella project, using the methods reported by the Air Quality Expert Group, may provide the most appropriate estimate of the proportion of oxides of nitrogen emitted as nitrogen dioxide.

The ADMS dispersion model will calculate the 99.8th percentile of hourly average nitrogen dioxide concentrations in rural areas, taking account of rural background monitoring data. However, short-term peak concentrations in urban areas are likely to be determined to a greater extent by low level emissions, mostly from road vehicles. The hourly mean objective is not generally exceeded at urban background monitoring sites in the UK. For the purposes of mapping at background locations, the 99.8th percentile concentrations may be estimated from the mapped background (without large point sources) annual average nitrogen dioxide concentrations using a statistical relationship of the form:

$$C_{99.8} = kC_{av}$$

where the constant k is determined from monitoring results and is typically 2-3.

Figure 4.14 shows the 99.8th percentile hourly average nitrogen dioxide concentration plotted against annual mean concentrations for background sites throughout the UK for 2003.

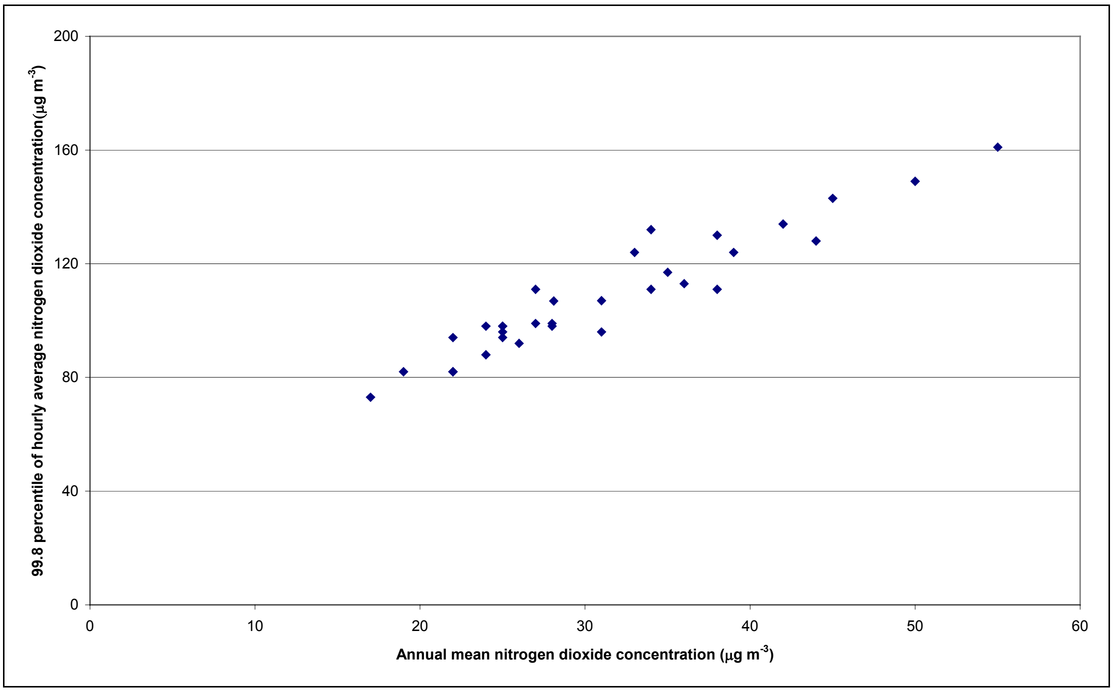


Figure 4.14: A plot of 99.8th percentile hourly average nitrogen dioxide concentration versus annual mean concentrations for urban background sites throughout the UK in 2003

The procedure described above yields two estimates of the 99.8th percentile hourly mean concentrations at each receptor point throughout the UK: one value resulting from the modelling of large point sources and the other based on the annual mean background concentration. The two sets of estimates may be combined to form a map of the larger of the two estimates at each receptor. This procedure assumes that short term-peak concentrations resulting from low level emissions do not coincide with peak concentrations associated with the large point sources: this assumption is reasonable because the meteorological conditions associated with high ground level concentrations are different in each case.

4.10.2 NO_x to NO_2 conversion

Use of the ADMS 3 chemistry module allows NO_x to NO_2 conversion to be taken directly into account. For the calculation of annual mean NO_2 concentrations, it is proposed to use the relationship:

$$[NO_2] = f\{NO_{x\_background}\} + 0.8NO_{x\_po\,\mathrm{int}\,source}$$

where $f\{NO_x\}$ is the AQEG relationship and the factor 0.8 takes account of the typical fraction converted for an elevated source (see Figure 4.5). Further development of the proposed method may take place as the result of other studies within the Environment Agency umbrella projects.

4.10.3 Improved input data quality

Potential improvements in the quality of the input data have been described for sulphur dioxide and apply equally for nitrogen dioxide.

The Netcen methodology for oxides of nitrogen currently assumes that emissions are constant throughout the year. For coal-fuelled power stations, the load factors shown in Table 3.2 can be used in the absence of local data. Gas-fuelled power stations usually provide base load and operate continuously at a high load factor. Other large industrial plants also tend to operate at near constant loading.

4.10.4 Long-range effects on annual mean concentrations

The Netcen methodology does not take account of the contribution to annual mean concentrations from large sources regulated by the Environment Agency that are over (typically) 50 km from the receptor locations. The Environment Agency needs to estimate the contribution from these sources to oxides of nitrogen concentrations at more distant receptors for the purposes of annual audit.

Oxides of nitrogen react in the atmosphere to form nitrate aerosols. The relative proportions of nitric oxide, nitrogen dioxide and other oxides of nitrogen approach equilibrium. The rate of loss of oxides of nitrogen by reaction is relatively slow, generally with a time constant of the order of 10 hours, and is thus relatively unimportant over distances of 100 km or less. However, at longer distances this loss of oxides of nitrogen may become significant. A number of models have been developed to take account of the loss by chemical reaction over long distances in predictions of acid deposition. Straight-line trajectory models such as HARM and TRACK have been used extensively in the UK to predict acid deposition.

For the purposes of this project, the acid deposition model TRACK was used to predict the contributions to annual average nitrogen oxide concentrations from large point sources greater than 50 km from each receptor and from area sources greater than 30 km from the receptor. ADMS 3 was used to predict the contribution from these sources closer to the receptor. A small change was made to the TRACK model code to prevent double counting of emissions within 50 km or 30 km of the receptor locations.

The TRACK model uses the Lagrangian trajectory approach, where species concentrations and depositions at receptors are the outcome of a windrose-weighted sum of contributions from straight-line trajectories centred on regular points of the compass. The original TRACK model assumed that each trajectory had a fixed cross-wind width, centred on the midpoint of each wind direction sector. This approach led to a ‘star pattern’ of predicted concentrations around large point sources. A small change was made to the TRACK model code so that emissions from across the whole of each wind direction sector would be taken into account (Appendix 8).

5 Netcen method for particulate matter, PM_{10}

Netcen prepared national scale maps of particulate matter (PM_{10}) concentrations for comparison with the air quality objectives and limit values presented in Table 5.1.

Table 5.1: Air quality limit values and objectives for PM_{10}

Pollutant	Air quality objective		Date to be achieved by
Particles (PM_{10}) (gravimetric)[c]			
24-hour limit value for the protection of human health	50 µg/m^3 not to be exceeded more than 35 times a year	24-hour mean	1.1.2005
Annual limit value for the protection of human health	40 µg/m^3	annual mean	1.1.2005
24-hour limit value for the protection of human health (except London)	50 µg/m^3 not to be exceeded more than seven times a year	24-hour mean	31.12.2010
24-hour limit value for the protection of human health (London)	50 µg/m^3 not to be exceeded more than 10 times a year	24-hour mean	31.12.2010
Annual limit value for the protection of human health (except Scotland and London)	20 µg/m^3	annual mean	31.12.2010
Annual limit value for the protection of human health (London)	23 µg/m^3	annual mean	31.12.2010
Annual limit value for the protection of human health (Scotland)	18 µg/m^3	annual mean	31.12.2010

The method assumes that the PM_{10} concentration comprises three components:

- primary combustion PM_{10}
- secondary PM_{10}
- 'other' PM_{10} (the residual).

Dispersion modelling methods are used to estimate the primary component alone. The secondary and other contribution is determined from the analysis of measured data.

Netcen only modelled annual average PM_{10} concentrations directly for comparison with the air quality objectives and limit values. Areas where the 24-hour daily mean limit value for 2005 would be exceeded were then identified by means of a statistical relationship between the number of exceedences and the annual mean. However, Netcen considered that the statistical relationship was not sufficiently robust to determine where the more stringent daily mean objectives for 2010 would be met.

5.1 Emissions estimates and discharge conditions

All Part A processes included within the National Atmospheric Emission Inventory with emissions greater than 200 tonnes per annum were included in the detailed dispersion modelling study to assess the primary component.

Prior to the modelling exercise, a survey of Part A authorisation notices held by the Environment Agency was conducted for all point sources with annual emissions greater than 200 tonnes as identified in the 2001 NAEI. Parameters characterising the release to atmosphere were collected; these were:

- stack height
- stack diameter
- discharge velocity
- discharge temperature.

Where release parameters were unavailable, engineering assumptions were applied. Previously collated data sets on emission release parameters from large SO_2 point sources were also used to characterise the release of emission (Abbott and Vincent, 1999).

Many of the Part A processes emit particulate matter through multiple stacks. We have ignored the possible enhancement of plume rise that may occur when plumes combine from stacks that are located near to each other. Where there are many stacks at the same site with different discharge conditions, for example at refineries or chemical works, we have, in some cases, grouped stacks of similar height and discharge characteristics together and assumed that the emission from each group of stacks may be represented by a single stack with characteristics of the stack with the largest emission or by a stack with an emission-weighted ‘average’ stack.

Power stations do not produce electricity at a constant rate, with electricity generation increasing and decreasing with demand. However, a constant emission rate was assumed for the purposes of modelling annual average particulate matter concentrations.

Emissions of smaller industrial sources regulated by the Environment Agency with emissions of less than 200 tonnes per annum were obtained from the NAEI on a 1 km x 1 km basis. The NAEI provides no details of the discharge conditions from these smaller industrial sources of particulate emissions. It was therefore assumed that the discharge height met the requirements of the Chimney Heights Memorandum, 3rd edition for oxides of nitrogen and that the mass emission rates of oxides of nitrogen (as nitrogen dioxide) and particulate matter were the same. Other assumptions included a discharge temperature of $100^{o}C$, a discharge velocity of $10\ m\ s^{-1}$, an emission factor of $0.1\ g\ MJ^{-1}$ and oxides of nitrogen (and particulate matter PM_{10}) concentrations in the discharge of $300\ mg\ m^{-3}$ at reference conditions. Further details are provided in Appendix 2.

Estimates of emissions from domestic, transport, Part B industrial sources and other area sources were obtained from the NAEI for each three km square area. Emissions from each road transport source were assumed to be distributed uniformly through an initial height of 10 m, where each three km source was represented by an emitting volume 3 km x 3 km square and 10 m high. The estimate of 10 m is based on the height of a typical house and assumes that road transport emissions will be entrained in the wake of nearby buildings. For other area sources, it was assumed that the initial emitting volume was 30 m high, corresponding to buoyant emissions from discharge stacks at small industrial or institutional premises. For road transport, it was assumed that the emissions varied throughout the week according to a profile obtained from an analysis of the distribution of all traffic in the United Kingdom by time of day (Road Traffic Statistics, 1999, Department of Transport) (see Figure 4.1). A constant rate of emission was assumed for other area sources.

National Atmospheric Emission Inventory estimates of aircraft emissions include emissions throughout the whole of the take-off and landing cycle. Only a small part of the emission is released near ground level and contributes to ground level oxides of nitrogen concentrations. A factor of 0.5 was applied to the aircraft emissions, representing that fraction emitted near to the ground. Similarly, factors of 0.25 and 0.5 are applied to NAEI estimates of shipping and quarry emissions.

5.2 Dispersion modelling

The dispersion modelling methods applied by Netcen to estimate the primary contribution to background particulate matter PM_{10} concentrations from large and small industrial sources and domestic, commercial and transport sources are the same as those used to predict the contribution to oxides of nitrogen concentrations from these sources.

5.3 Secondary particulate concentrations

Sulphate and nitrate particle concentrations are measured on a monthly basis at 12 rural sites in the ammonia and nitric acid network using a denuder method (CEH, 2003). For simplicity, secondary particles were assumed to consist of sulphates and nitrates only.
The secondary component of PM_{10} was estimated from:

$$[PM_{10}]_{secondary} = a \times [SO_4^{2-}] \; + b \times [NO_3^-]$$

where:

- $[PM_{10}]_{secondary}$ is the secondary contribution to the PM_{10} concentration measured by tapered element oscillating microbalance (TEOM);
- $[NO_3^-]$ is the measured nitrate aerosol concentration;
- $[SO_4^{2-}]$ is the measured sulphate aerosol concentration;
- a and b are mass conversion factors that depend to some extent on the methods used to measure the PM_{10} concentration.

Sulphate particulate concentrations are also measured on a daily basis at five monitoring sites in the acid deposition network. The daily data was used to estimate the mass conversion factors as follows.

There are 11 sites in the automatic and urban rural network where PM_{10} concentrations and oxides of nitrogen concentrations are both measured continuously. An assessment of the daily concentration measurements at each site is carried out using the regression model suggested by APEG:

$$[PM_{10}] = A \times [NO_x] + B \times [SO_4^{2-}] + C$$

where:

A, B and C are empirical constants determined separately for each site;
$[PM_{10}]$ is the daily average PM_{10} concentration measured by tapered element oscillating microbalance (TEOM) at the site;
$[NO_x]$ is the daily average NO_x concentration measured at the site;
$[SO_4^{2-}]$ is the daily average sulphate concentration measured at the nearest acid deposition network site.

The three terms on the right hand side of the regression model equation correspond to the primary, secondary and other particulate components of the measured PM_{10} concentration.

Table 5.2 shows the regression model coefficients for 1996 data reported for eight sites in the APEG report.

Table 5.2: Empirical coefficients used to predict PM_{10} concentrations

	A (primary)	B (secondary)	C (other)
London Bloomsbury	0.112	2.55	9.29
Birmingham Centre	0.207	2.29	6.52
Bristol Centre	0.145	2.62	7.97
Manchester Piccadilly	0.160	2.95	7.69
Newcastle Centre	0.155	3.48	5.66
Belfast Centre	0.302	2.65	5.91
Edinburgh centre	0.122	2.99	6.42
Liverpool Centre	0.187	2.56	7.57

Typically, the average value of the receptor coefficient B is in the range 2-3, changing on a year to year basis and spatially as the proportions of sulphate and nitrate change.

It is then assumed that the daily average sulphate and nitrate concentrations are correlated at each site so that the APEG receptor coefficient:

$$B = a + b\frac{[NO_3^-]_{average}}{[SO_4^{2-}]_{average}}$$

where a and b are constants and $[\ ]_{average}$ denotes average sulphate and nitrate concentrations interpolated from the ammonium and nitric acid network.

The constant a was determined on the assumption that sulphate aerosol was largely present as ammonium sulphate and that both the ammonium and sulphate ions contributed fully to the measured concentration: thus a = 1.354.

It was also assumed that nitrate aerosol was largely present as ammonium nitrate: however, TEOM instruments are known to be subject to partial losses of the more volatile particle components, such as ammonium nitrate. The constant b was therefore determined from the regression analysis by subtraction:

$$b = (B - a)\frac{[SO_4^{2-}]_{average}}{[NO_3^-]_{average}}$$

Typically b is approximately unity: this value may be compared with a value of 1.29 that would apply if all the nitrate were present as ammonium nitrate and there were no losses of volatile matter in the TEOM device.

A map of secondary PM_{10} particle concentrations across the UK was then calculated from the ammonia and nitric acid network measurements of sulphate and nitrate concentrations by interpolation onto a 20 km x 20 km grid, assuming mass correction factors of a = 1.354 and b = 1.0 for sulphate and nitrate respectively:

$$[PM_{10}]_{secondary} = a \times [SO_4^{2-}] + b \times [NO_3^-]$$

Air quality objectives for PM_{10} are specified in terms of the gravimetric reference standard method rather than the TEOM device. The gravimetric device behaves differently from the TEOM device so that receptor coefficients and mass correction factors derived using TEOMs may not apply. There are now a limited number of gravimetric devices installed in the UK, but the analysis to determine the equivalent receptor coefficients at these sites has not yet been done.

5.4 Relationship between gravimetric and tapered element oscillating microbalance measurements of PM_{10} concentrations

The reference method to compare measured concentrations with the limit values for PM_{10} is the use of a gravimetric instrument. The analysis developed by Netcen is based on TEOM (tapered element oscillating microbalance) instruments, which are currently widely used within UK national monitoring networks. Netcen applied a scaling factor of 1.3 to all data before comparing with the limit value, as suggested by APEG (1999), and recommended as an interim measure by the EC Working Group set up to address the issue of scaling automatic PM_{10} measurements in advance of Member States undertaking their own detailed inter-comparisons with the Directive Reference Method.

5.5 Area source calibration

Modelled PM_{10} concentrations were then compared with those obtained at rural, suburban, urban background and urban centre monitoring sites in Defra’s automatic and urban rural network. Modelled contributions from large and small point sources and interpolated secondary concentrations were subtracted from the measured concentrations: the remainder was then compared with the modelled contribution from area sources. Figure 5.1 shows this remainder plotted against the modelled prediction of the area source contribution.

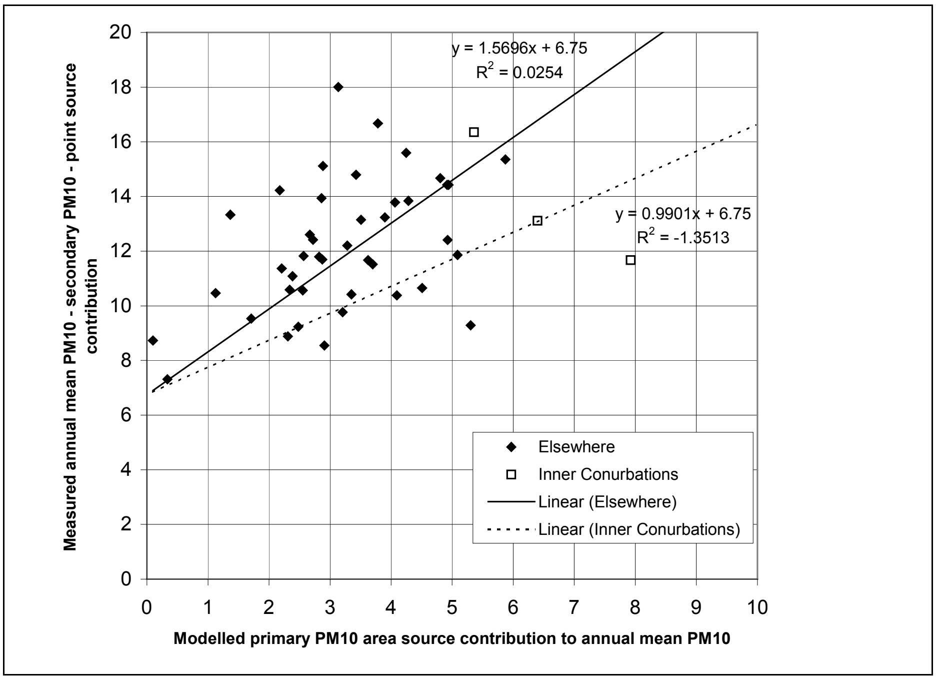


Figure 5.1: Calibration of PM_{10} area source model

Figure 5.1 shows that measured residual concentrations are higher than the modelled area source contribution. In each case, the difference is at least 6.75 μg m^{-3} (TEOM). It has been assumed that this offset is representative of coarse or other particulate sources. In practice, the coarse or other particulate contribution is very uncertain because it is affected to a great extent by local circumstances, such as the type of soil or frequency of road sweeping. The uncertainty in the coarse or other component is comparable in size to the primary contribution, so that the plotted points in Figure 5.1 show considerable scatter.

Netcen divided the monitoring sites into two groups, following the analysis for oxides of nitrogen:

- inner conurbations
- elsewhere.

'Inner conurbations' includes inner and central London and central Birmingham and Manchester as defined by DfT (2003). Regression analysis was applied to the two groups of data to determine calibration slopes.

The modelled area source contribution was multiplied by the relevant empirical slope to calculate the calibrated area source contribution for each grid square in the country. The modelled point source, mapped secondary particle concentrations and the estimated coarse or other component were then added to the area source contribution to provide mapped annual mean values over the whole country.

5.6 Roadside concentrations

Netcen also developed empirical techniques for the estimation of roadside PM_{10} concentrations similar to those used for oxides of nitrogen. The annual mean concentration of PM_{10} at a roadside location is made up of two parts: the background concentration (as described above) and a roadside increment:

Roadside PM_{10} concentration = background PM_{10} concentration + PM_{10} roadside increment

The roadside increment was estimated at roadside monitoring stations; the background PM_{10} component was derived from the map described above and subtracted from the measured roadside PM_{10} concentration.

The NAEI provides estimates of PM_{10} emissions for major road links in the UK. Netcen have assumed that the roadside increment is related to the emission per unit length of road, E, by means of a relationship of the form:

$$PM_{10}\_roadside\_increment = kfE$$

where:

k is an empirical constant for PM_{10}, typically 0.24 s m^{-2};
f is an empirical adjustment factor that takes account of the annual average daily traffic flow and the type of road.

The empirical constant k is larger for PM_{10} than for NO_x: this may be because the NAEI inventory does not take account of the contribution from re-suspended dust to roadside concentrations.

5.7 Frequency of exceedence of the daily mean limit value

The methods described above allow Netcen to prepare maps of annual average PM_{10} concentrations. Stedman has analysed data from monitoring stations throughout the country over the period 1992-1999. Figure 5.2 shows the number of exceedences of the 50 μg m^{-3} 24-hour standard plotted against the annual mean (gravimetric) concentration. An annual mean concentration of 31.5 μgm^{-3} gravimetric has been taken to be equivalent to 35 days with 24-hour mean concentrations greater than 50 μg m^{-3} gravimetric (the stage 1 24-hour limit value). Figure 5.2 also shows that the annual average objectives for 2010 are likely, on the basis of recent measurements, to be at least as stringent as the 24-hour objectives. Netcen has therefore not assessed mapped PM_{10} concentrations against the 2010 objectives.

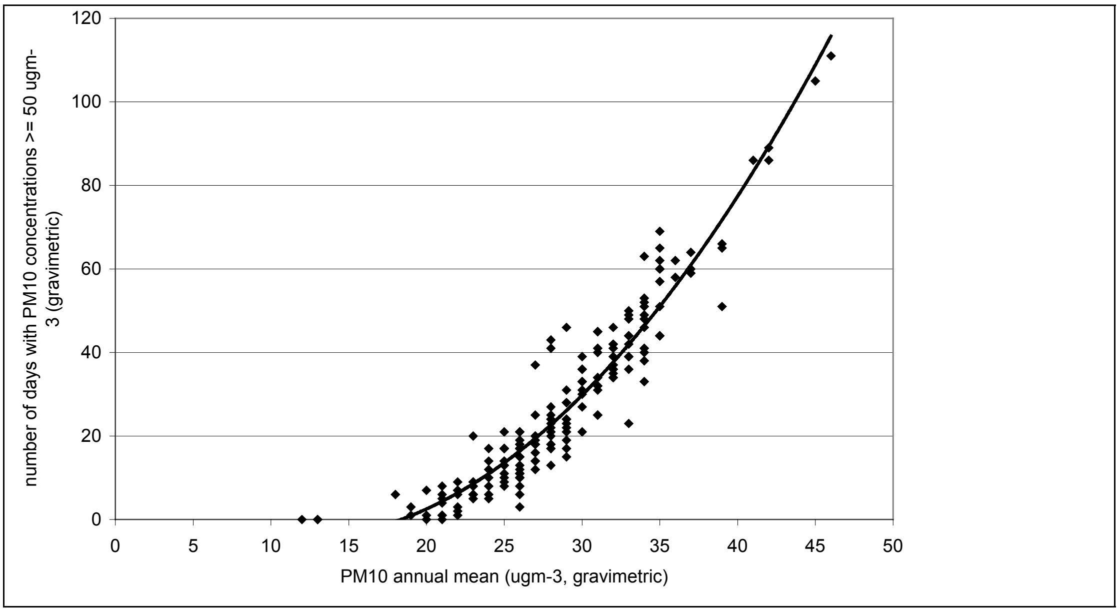


Figure 5.2: Relationship between the number of days with PM_{10} concentrations greater than or equal to 50 μg m^{-3} and annual mean concentration (1992 –1999)

5.8 Model verification

Modelled annual average PM_{10} concentrations were compared with measured concentrations at monitoring sites throughout the UK. The sites used in the verification process include sites other than those in Defra's automatic urban and rural network. Data from sites quality assured by Netcen under contract but not part of the national network, including local authority sites in the Netcen Calibration Club, have therefore been used for the verification of modelled estimates. The term 'verification sites' is used to describe all monitoring sites included in the verification analysis. The monitoring sites used for this comparison are listed in Appendix 6. Sites with a data capture of at least 50 per cent were included in the verification analysis. A higher data capture threshold of 75 per cent was applied for the national network sites used to calibrate the models.

Figure 5.3 and Figure 5.4 show verification plots of measured and modelled PM_{10} concentrations at background and roadside monitoring sites.

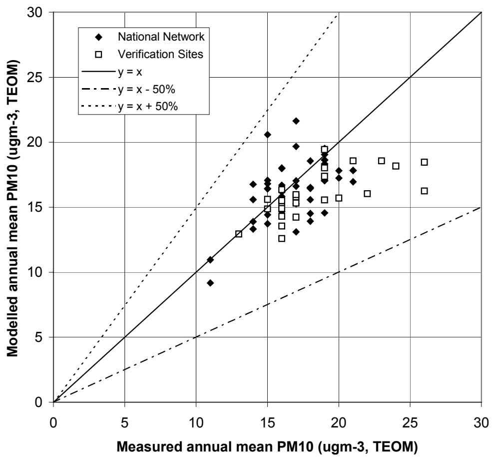


Figure 5.3 Verification of background annual mean PM_{10} model 2002

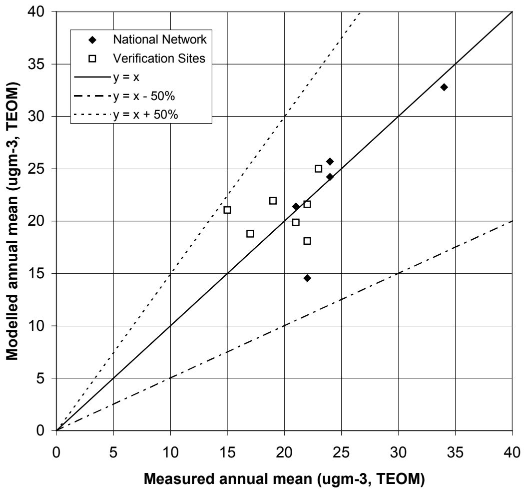


Figure 5.4 Verification of roadside annual mean PM_{10} model 2002

5.9 Mapped concentrations

Figure 5.5 and Figure 5.6 show the empirical map produced by Netcen of background and roadside annual mean PM_{10} concentrations for 2002.

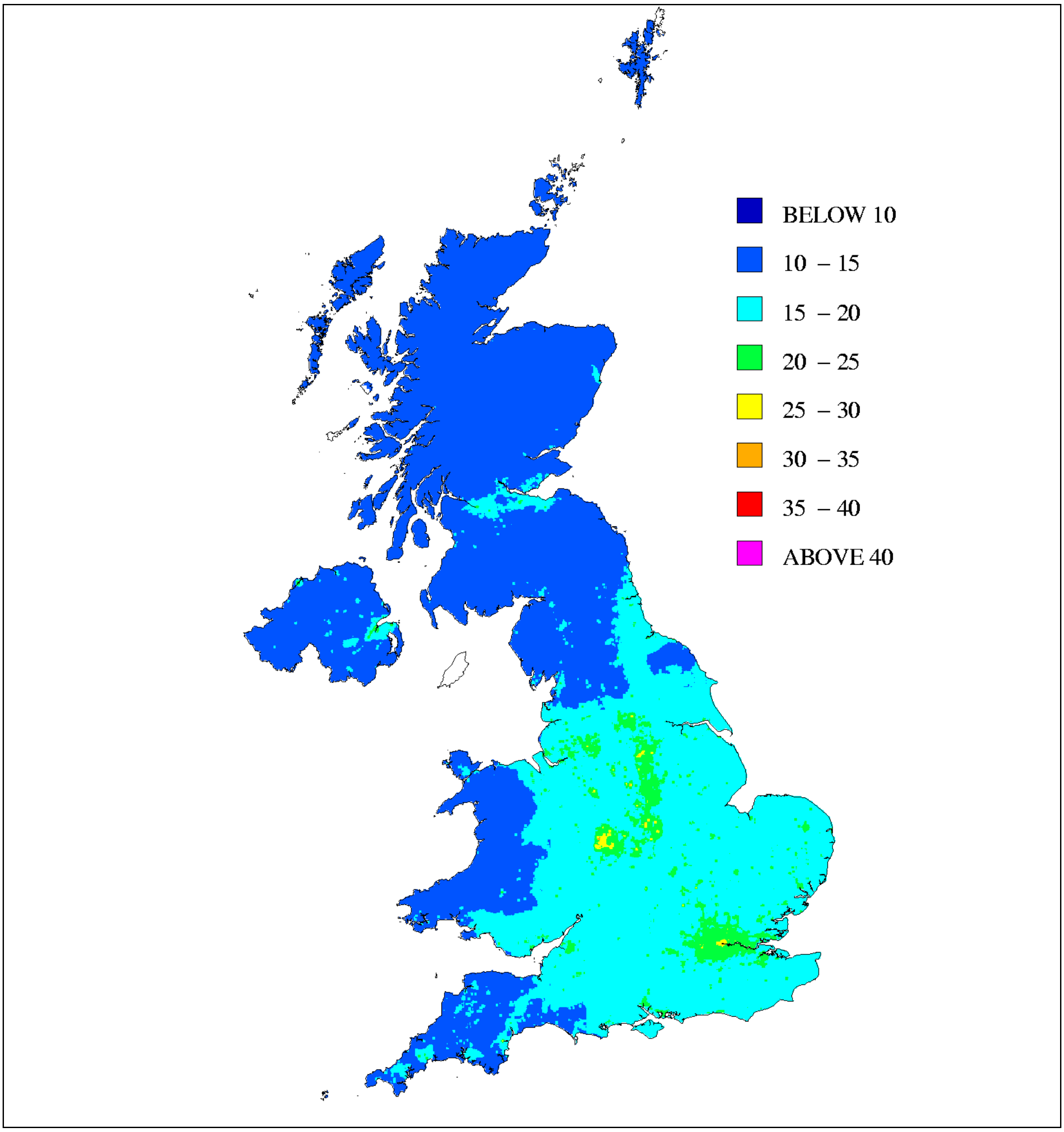


Figure 5.5: Annual mean background PM$_{10}$ concentration, 2002 (μg m^{-3}, gravimetric). Concentrations are predicted for 1 km x 1 km squares.

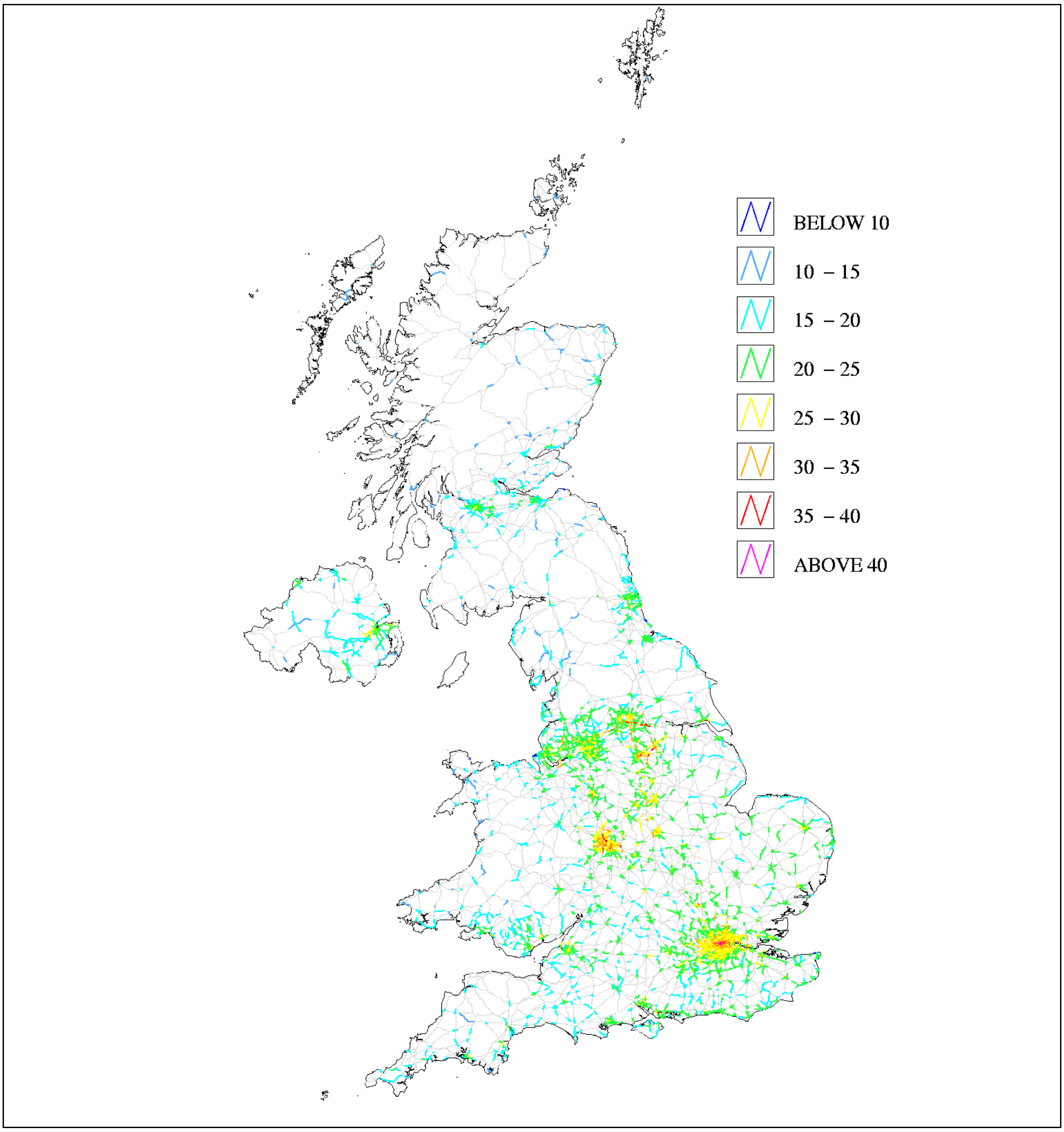


Figure 5.6: Major built-up roads, annual mean roadside PM_{10} concentration, 2002 ($\mu g\ m^{-3}$, gravimetric)

5.10 Model development

A number of potential improvements to the method, similar to those for sulphur dioxide and nitrogen dioxide, would increase its utility in assessing the contribution of processes regulated by the Environment Agency to particulate matter concentrations for the purposes of annual audit. These include:

- improved input data quality;
- increased modelling resolution;
- assessment of long-range effects of Environment Agency-regulated emissions on annual mean concentrations;
- more consistent treatment of background concentrations;

- assessment of prediction intervals for modelled concentrations;
- spatial analysis of residual errors
- preparation of incremental maps
- site-specific studies for areas where large pollutant concentrations are predicted or measured.

Specific developments relating to particulate matter modelling are described in the following sections.

5.10.1 Long-range effects on annual mean concentrations

The Netcen methodology does not take account of the contribution to annual mean concentrations from large sources regulated by the Environment Agency that are over (typically) 50 km from the receptor locations. The Environment Agency needs to estimate the contribution from these sources to particulate matter concentrations at more distant receptors for the purposes of annual audit.

Emissions from Environment Agency-regulated sources may contribute to particulate matter concentrations in two ways:

- emissions of particulate matter contribute directly to the primary particulate matter concentration;
- emissions of sulphur dioxide and oxides of nitrogen react in the atmosphere to form sulphate, nitrite and nitrate aerosols which contribute to secondary particulate matter concentrations.

The rate of particulate formation by reaction is relatively slow and is relatively unimportant over distances of 100 km or less. However, at longer distances the secondary component by reaction may become significant. A number of models have been developed to take account of the secondary formation by chemical reaction over long distances in predictions of acid deposition. Straight-line trajectory models such as HARM and TRACK have been used extensively in the UK to predict acid deposition.

For the purposes of this project, the acid deposition model TRACK was used to predict the contribution from sulphur dioxide and oxides of nitrogen emissions to particulate matter concentrations.

6 Proposed method for long-term sulphur dioxide objectives

This section outlines the proposed method for assessing the contribution made by Environment Agency-regulated sources to long-term objective limits for sulphur dioxide.

6.1 Scenarios

Develop model scenarios:

- current year
- future year (National Emissions Ceiling Directive).

6.2 Emissions and discharge characteristics

Identify emissions sources emitting more than 500 tonnes of sulphur dioxide per annum.
Review available data on emissions and temporal variation of emissions.
Review available data on discharge characteristics and their temporal variation.

Obtain most up-to-date area source inventory from the NAEI.
Obtain 50 km x 50 km gridded 'expert' emissions data for the EMEP area for relevant source sectors from EMEP web site (http://webdab.emep.int/).

6.3 Point source dispersion model input files

Define 100 x 100 km receptors areas for each emission source.
Prepare time-varying files for each point source containing details of emissions, discharge temperature and discharge velocity temporal variation.
Specify meteorological data (Waddington sequential hourly data for most recent year).
Prepare dispersion model (ADMS 3) main input files containing details of stack heights and diameters and so on, for each emissions source.

Default input data for each receptor area includes:

Parameter	Value
Surface roughness	0.1 m
Dry deposition velocity	ADMS 3 default value for a reactive gas
Wet deposition $\Lambda = AP^B$	Default values $A = 10^{-4}\ s^{-1}$, $B = 0.64$, P is precipitation in mm h^{-1} ADMS 3 limits wet deposition for sulphur dioxide on the basis of the pH of rain drops
Receptor grid	2 km x 2 km intervals covering area extending 100 km x 100 km centred on each source
Specific heat of discharge	1012 J $^{o}C^{-1}$ kg^{-1} (default)
Molecular weight of discharge	28.96 (default)
Meteorological data	Hourly sequential in 10^{o} sectors Use model default advanced meteorological parameters
Outputs	99.9th percentile 15-minute average 99.73th percentile hourly average 99.18th percentile 24-hour average annual average

Run the model to provide output files with predicted annual mean concentration at each receptor. Modelled percentile concentrations are not used for maps but may be used to assess contribution from individual sources to exceedences of short-term objective limits.

6.4 Area source dispersion model kernel

Prepare 1 km x 1 km dispersion model kernels using ADMS3. The source-receptor relationship for the central node of the kernel is modified so that emissions within 50 m of a background receptor location are not taken into account: the emissions from a 100 m x 100 m square surrounding the receptor are reallocated throughout the rest of the 1 km x 1 km square (see Figure 6.1).

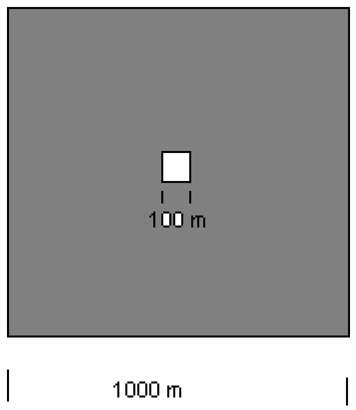


Figure 6.1: Reallocation of emissions around the central node of the kernel

Parameter	**Value**
Emission area coordinates, m	{-500,-500} {500,-500} {500, 500} {-500, 500}
Volume source depth	10 m
Emission rate	1 g/s
Receptor area coordinates, m	{-30000,-30000} {30000, 30000}
Surface roughness	1 m
Dry deposition velocity	0
Wet deposition	0
Molecular weight of discharge	28.96 (default)
Met data	Hourly sequential in 10^{o} sectors Use model default advanced meteorological parameters
Outputs	Annual mean

Run model to provide output kernels. Prepare small industrial source kernel (Appendix 2).

6.5 Area source modelling

Obtain 1 km x 1 km area source emissions data from NAEI.

Use ArcInfo 'focal sum' function to multiply each area source emission by the appropriate factor in the dispersion kernel and sum the contributions from each emission source at the centroid of each 1 km x 1 km receptor square.

6.6 Long-range modelling

Prepare 50 km EMEP grid emission input files from EMEP inventory for relevant source sectors.

Obtain 1 km x 1 km gridded sulphur dioxide area source data from NAEI. Obtain point source emission data for relevant source sectors from NAEI. Aggregate source data onto a 10 km x 10 km grid.

Run TRACK model. Model version 1.6f excludes the contribution from elevated sources greater than 50 km from receptors and from low level sources greater than 30 km from receptors.

Other input parameters are as follows:

Parameter	Value
Receptor grid	Ordnance survey
Receptor square dimension	20 km
Stability class	4
Mean wind speed	7.5 m s $^{-1}$
Trajectory duration	96 hours
Trajectory time step	120 seconds
Lookup time step	2,880 seconds
Number of incoming trajectories at receptor	24
Number of trajectories per 24-hour period	4
Choice of solver	Fixed timestep
Number of vertical levels	Single level
Deposition velocities	Spatially disaggregated values based on surface types (Table 3.6)
Choice of season	All year
Seeder-feeder enhancement	On
Seeder-feeder effect cut-in level	800 mm rain per year
Seeder-feeder factor on wet deposition rate	2
Seeder-feeder factor on sulphur dioxide oxidation rate	1.3
Tracer	Off
Source type	Area sources

6.7 Model calibration

Identify rural and power company monitoring stations with the year's ratified data and with more than 75 per cent data capture. Derive annual and winter means.

Obtain the following:

- nearest neighbour prediction from point source dispersion modelling at each monitoring station;
- nearest neighbour prediction from area source modelling at each monitoring station;
- nearest neighbour prediction from long-range modelling at each monitoring station.

Carry out analysis to obtain calibration factors based on a regression model of the form:

$$c_{measured} = A(c_{\mathrm{mod}elled\_industrial} + c_{\mathrm{mod}elled\_area} + c_{long\_range}) + B$$

where A and B are constants determined by the regression analysis.

Determine prediction intervals (see Section 3.6.5).

Calculate residuals at each of the calibration sites:

Residual = measured - regression model

Use kriging interpolation program (such as Surfer^{TM}) to prepare variograms of the residuals.

6.8 Prepare ArcInfo GIS maps

Interpolate point source and long-range model predictions onto 1 km x 1 km grid.

Add contributions from point sources, area sources and long-range sources by application of the calibration model.

Plot modelled concentrations as a map of the UK.

6.9 Verification

Compare modelled and measured concentrations at other monitoring stations not selected for calibration.

6.10 Map review

Identify monitoring stations where measured concentrations are outside model prediction interval and where the modelled or measured concentrations approach the air quality objective.

Identify map locations where the air quality objective concentration is within the model prediction interval.

Review model input data for sources potentially affecting the locations identified.

7 Proposed method for short-term sulphur dioxide objectives

This section outlines the proposed method for assessing the contribution made by Environment Agency-regulated sources to short-term objective limits for sulphur dioxide.

7.1 Scenarios

Develop model scenarios:

- current year
- future year (National Emissions Ceiling Directive).

7.2 Emissions and discharge characteristics

Identify emissions sources emitting more than 500 tonnes of sulphur dioxide per annum.
Review available data on emissions and temporal variation of emissions.
Review available data on discharge characteristics and their temporal variation.

Obtain most up-to-date area source inventory from the NAEI.

7.3 Point source dispersion model input files

Define receptors areas (see Figure 3.1).

Identify large emission point sources potentially affecting each receptor area.

Prepare time-varying files for each receptor area containing details of emissions, discharge temperature and discharge velocity temporal variation for each point source.

Specify meteorological data (Waddington sequential hourly data for most recent year).

Prepare dispersion model (ADMS 3) main input files for each receptor area containing details of stack heights and diameters and so on, for each emission source potentially affecting each receptor area.

Default input data for each receptor area includes:

Parameter	**Value**
Surface roughness	0.1 m
Dry deposition velocity	0^+
Wet deposition $\Lambda = AP^B$	0^+
Receptor grid	2 km x 2 km intervals covering defined area (Fig. 3.1)
Specific heat of discharge	1,012 J $^{o}C^{-1}$ kg^{-1} (default)
Molecular weight of discharge	28.96 (default)
Met data	Hourly sequential in 10° sectors Use model default advanced meteorological parameters
Outputs	99.9th percentile 15-minute average 99.73th percentile hourly average 99.18th percentile 24-hour average Annual mean

$^+$Wet and dry deposition at short range suppressed by hydrogen chloride in the plume.

Run model to provide output files.

7.4 Model calibration

Identify rural and power company monitoring stations with the year's ratified data and with more than 75 per cent data capture. Derive 99.9th percentile 15-minute means, 99.73th percentile hourly means, 99.18th percentile daily means and annual means.

Obtain nearest neighbour prediction from point source dispersion modelling at each monitoring station.

Obtain nearest neighbour prediction from annual average area source modelling at each monitoring station (from long-term modelling; see Section 6) .

Carry out analysis to obtain calibration factors based on a regression model of the form:

$$c_{measured} = \max\begin{bmatrix} Ac_{\mathrm{mod}elled\_industrial,\%ile} + 2(c_{\mathrm{mod}elled\_area} + c_{long\_range})_{annual} \\ 2Ac_{\mathrm{mod}elled\_industrial,annual} + k(c_{\mathrm{mod}elled\_area} + c_{long\_range})_{annual} \end{bmatrix}$$

where:

> k is a background multiplier factor relating background percentile concentrations to annual averages (11.0, 10.1 and 3.3 respectively for the 99.9th percentile 15-minute mean, 99.73th percentile hourly mean and 99.18th percentile daily mean values);
> A is a constant determined by the regression analysis.

Determine prediction intervals (see Section 3.6.5).

7.5 Prepare ArcInfo GIS maps

For each 1 km x 1 km grid square throughout the UK, carry out the following:

Interpolate point source model predictions of percentile concentrations onto 1 km x 1 km grid.

Add contributions from area sources and other sources by applying the calibration model.

Plot modelled concentrations as a map of the UK.

7.6 Verification

Compare modelled and measured concentrations at other monitoring stations not selected for calibration.

7.7 Map review

Identify monitoring stations where measured concentrations are outside model prediction interval and where the modelled or measured concentrations approach the air quality objective.

Identify map locations where the air quality objective concentration is within the model prediction interval.

Review model input data for sources potentially affecting the locations identified.

8 Proposed method for long-term oxides of nitrogen dioxide objectives

This section outlines the proposed method for assessing the contribution made by Environment Agency-regulated sources to long-term objective limits for oxides of nitrogen and nitrogen dioxide.

8.1 Scenarios

Develop model scenarios:

- current year
- future year (National Emissions Ceiling Directive).

8.2 Emissions and discharge characteristics

Identify emissions sources emitting more than 500 tonnes of nitrogen oxides per annum.
Review available data on emissions and temporal variation of emissions.
Review available data on discharge characteristics and their temporal variation.

Obtain most up-to-date area source inventory from the NAEI.
Obtain 50 km x 50 km gridded 'expert' emissions data for the EMEP area for relevant source sectors from EMEP web site (http://webdab.emep.int/).

8.3 Point source dispersion model input files

Define 100 x 100 km receptors areas for each emission source.
Prepare time-varying files for each point source containing details of emissions, discharge temperature and discharge velocity temporal variation.
Specify meteorological data (Waddington sequential hourly data for most recent year).
Prepare dispersion model (ADMS 3) main input files containing details of stack heights and diameters and so on, for each emissions source.

Default input data for each receptor area includes:

Parameter	**Value**
Surface roughness	0.1 m
Dry deposition velocity	0
Wet deposition $\Lambda = AP^B$	0
Receptor grid	2 km x 2 km intervals covering area extending 100 km x 100 km centred on each source
Specific heat of discharge	1,012 J $^{o}C^{-1}$ kg^{-1} (default)
Molecular weight of discharge	28.96 (default)
Met data	Hourly sequential in 10^{o} sectors Use model default advanced meteorological parameters
Outputs	99.8th percentile hourly average annual average
Chemistry module	Off

Run model to provide output files with predicted annual mean concentration at each receptor. Modelled percentile concentrations are not used for maps but may be useful to assess contribution from individual sources to exceedences of short-term objective limits.

8.4 Area source dispersion model kernel

Prepare 1 km x 1 km dispersion model kernels using ADMS 3. The source-receptor relationship for the central node of the kernel is modified so that emissions within 50 m of a background receptor location are not taken into account: the emissions from a 100 m x 100 m square surrounding the receptor are reallocated throughout the rest of the 1 km x 1 km square (see Figure 6.1).

Parameter	Value
Emission area coordinates, m	{-500,-500} {500,-500} {500, 500} {-500, 500}
Volume source depth	10 m
Emission rate	1 g/s
Receptor area coordinates, m	{-30000, -30000} {30000, 30000}
Surface roughness	1 m
Dry deposition velocity	0
Wet deposition	0
Molecular weight of discharge	28.96 (default)
Met data	Hourly sequential in 10^o sectors Use model default advanced meteorological parameters
Outputs	Annual mean
Chemistry module	Off

Run model to provide output kernels. Prepare small industrial source kernel (Appendix 2).

8.5 Area source modelling

Obtain 1 km x 1 km area source emissions data from NAEI.

Use ArcInfo 'focal sum' function to multiply each area source emission by the appropriate factor in the dispersion kernel and sum the contributions from each emission source at the centroid of each 1 km x 1 km receptor square.

8.6 Long-range modelling

Prepare 50 km EMEP grid emission input files from EMEP inventory for relevant source sectors.

Obtain 1 km x 1 km gridded oxides of nitrogen area source data from NAEI. Obtain point source emission data for relevant source sectors from NAEI. Aggregate source data onto 10 km x 10 km grid.

Run TRACK model. Model version 1.6f excludes the contribution from elevated sources greater than 50 km from receptors and from low level sources greater than 30 km from receptors.

Other input parameters are as follows:

Parameter	**Value**
Receptor grid	Ordnance survey
Receptor square dimension	20 km
Stability class	4
Meanwind speed	7.5 m s^{-1}
Trajectory duration	96 hours
Trajectory timestep	120 seconds
Lookup timestep	2,880 seconds
Number of incoming trajectories at receptor	24
Number of trajectories per 24-hour period	4
Choice of solver	Fixed timestep
Number of vertical levels	Single level
Deposition velocities	Spatially disaggregated values from input file
Choice of season	All year
Seeder-feeder enhancement	On
Seeder-feeder effect cut-in level	800 mm rain per year
Seeder-feeder factor on wet deposition rate	2
Seeder-feeder factor on sulphur dioxide oxidation rate	1.3
Tracer	Off
Source type	Area sources

8.7 Model calibration

Identify rural, urban background and power company monitoring stations with the year's ratified data and with more than 75 per cent data capture. Derive annual and winter means.

Obtain the following:

- nearest neighbour prediction from point source dispersion modelling at each monitoring station;
- nearest neighbour prediction from area source modelling at each monitoring station;
- nearest neighbour prediction from long-range modelling at each monitoring station.

Carry out an analysis to obtain calibration factors based on a regression model for NO_x of the form:

$$c_{measured} = A(c_{\mathrm{mod}elled\_industrial} + c_{\mathrm{mod}elled\_area} + c_{long\_range})$$

where A is a constant determined by the regression analysis.

Determine prediction intervals (see Section 3.6.5).

8.8 Calculation of nitrogen dioxide concentrations

For the calculation of annual mean NO_2 concentrations, use the relationship:

$$[NO_2] = f\{NO_{x\_background}\} + 0.8NO_{x\_po\,\mathrm{int}\,source}$$

where f{NO_x} is the AQEG relationship and the factor 0.8 takes account of the typical fraction converted for an elevated source (see Figure 4.5). Further development of the proposed method may take place as the result of other studies within the Environment Agency umbrella projects.

8.9 Prepare ArcInfo GIS maps

For each 1 km x 1 km grid square centroid throughout the UK, carry out the following:

Interpolate point source model predictions of percentile concentrations onto 1km x 1 km grid.

Add contributions from area sources, long-range sources and other sources by application of the calibration model.

Plot modelled concentrations as a map of the UK.

8.10 Verification

Compare modelled and measured concentrations at other monitoring stations not selected for calibration.

8.11 Map review

Identify monitoring stations where measured concentrations are outside model prediction interval and where the modelled or measured concentrations approach the air quality objective.

Identify map locations where the air quality objective concentration is within the model prediction interval.

Review model input data for sources potentially affecting the locations identified.

9 Proposed method for short-term nitrogen dioxide objectives

This section outlines the proposed method for assessing the contribution made by Environment Agency-regulated sources to short-term objective limits for nitrogen dioxide.

9.1 Scenarios

Develop model scenarios:

- current year
- future year (National Emissions Ceiling Directive).

9.2 Emissions and discharge characteristics

Identify emissions sources emitting more than 500 tonnes of oxides of nitrogen per annum.
Review available data on emissions, temporal variation of emissions.
Review available data on discharge characteristics and their temporal variation.

Obtain most up-to-date area source inventory from the NAEI.

9.3 Point source dispersion model input files

Define receptors areas (see Figure 3.1).

Identify large emission point sources potentially affecting each receptor area.

Prepare time-varying files for each receptor area containing details of emissions, discharge temperature and discharge velocity temporal variation for each point source.

Prepare background pollutant concentration files for model year (ozone, nitrogen dioxide, nitric oxide) from a representative monitoring station.

Specify meteorological data (Waddington sequential hourly data for the same year as the background data).

Prepare dispersion model (ADMS 3) main input files for each receptor area containing details of stack heights and diameters and so on, for each emissions source potentially affecting each receptor area.

Default input data for each receptor area includes:

Parameter	**Value**
Surface roughness	0.1 m
Dry deposition velocity	0
Wet deposition $\Lambda=AP^B$	0
Chemistry	Simple chemistry scheme on for nitrogen dioxide modelling and off for oxides of nitrogen modelling
Receptor grid	2 km x 2 km intervals covering defined area (Fig. 3.1)
Specific heat of discharge	1,012 J $^oC^{-1}$ kg^{-1} (default)
Molecular weight of discharge	28.96 (default)
Met data	Hourly sequential in 10^o sectors Use model default advanced meteorological parameters
Outputs	99.8th percentile of hourly means of oxides of nitrogen and nitrogen dioxide concentrations

Run model to provide output files.

.

9.4 Model calibration

Identify rural and power company monitoring stations with the year's ratified data and with more than 75 per cent data capture. Derive 99.8th percentile of hourly means of oxides of nitrogen concentrations and nitrogen dioxide concentrations.

Obtain estimated annual mean nitrogen dioxide concentrations at each monitoring station (see Section 4.9).

Select monitoring stations where the 99.8th percentile of nitrogen dioxide concentrations exceeds three times the estimated annual mean.

Carry out analysis of 99.8th percentile data for selected monitoring stations to obtain calibration factors based on a regression model of the form:

$$c_{measured} = Ac_{\mathrm{mod}elled\_industrial} + B$$

where

A is a constant determined by the regression analysis;
B is a constant variously determined by the regression analysis or on the basis of a priori judgement.

Determine prediction intervals (see Section 3.6.5).

9.5 Prepare ArcInfo GIS maps

For each 1 km x 1 km grid square centroid throughout the UK, carry out the following:

Interpolate point source model predictions of percentile concentrations onto 1 km x 1 km grid,

Apply the calibration model to each grid node.

Obtain the estimated annual average nitrogen dioxide concentration at each point (see Section 8).

Plot maximum of (calibrated point source model, three times the annual mean).

9.6 Verification

Compare modelled and measured concentrations at other monitoring stations not selected for calibration.

9.7 Map review

Identify monitoring stations where measured concentrations are outside model prediction interval and where the modelled or measured concentrations approach the air quality objective.

Identify map locations where the air quality objective concentration is within the model prediction interval.

Review model input data for sources potentially affecting the locations identified.

9.8 Detailed modelling of identified locations

Obtain additional data on emissions, discharge characteristics, buildings, meteorology and topography.

Use ADMS 3 dispersion model to predict pollutant concentrations, taking account of new data. Reassess risk of exceeding air quality objective.

10 Proposed method for particulate matter objectives

This section outlines the proposed method for assessing the contribution made by Environment Agency-regulated sources to objective limits for particulate matter, PM_{10}.

10.1 Scenarios

Develop model scenarios:

- current year
- future year (National Emissions Ceiling Directive).

10.2 Emissions and discharge characteristics

Identify emissions sources emitting in excess of 500 tonnes of oxides of nitrogen, 500 tonnes of sulphur or 100 tonnes of particulate matter PM_{10} per annum.
Review available data on emissions and temporal variation of emissions.
Review available data on discharge characteristics and their temporal variation.

Obtain most up-to-date area source inventory from the NAEI.
Obtain 50 km x 50 km gridded 'expert' emissions data for the EMEP area for relevant source sectors from EMEP web site (http://webdab.emep.int/).

10.3 Point source dispersion model input files

Define 100 x 100 km receptors areas for each PM_{10} emission source.

Prepare time-varying files for each point source containing details of emissions, discharge temperature and discharge velocity temporal variation.

Specify meteorological data (Waddington sequential hourly data for most recent year).

Prepare dispersion model (ADMS 3) main input files containing details of stack heights and diameters and so on, for each emissions source.

Default input data for each receptor area includes:

Parameter	Value
Surface roughness	0.1 m
Dry deposition velocity	0.001 m/s
Wet deposition $\Lambda = AP^B$	A = 10^{-4} s^{-1}, B = 0.64
Receptor grid	2 km x 2 km intervals covering area extending 100 km x 100 km centred on each source
Specific heat of discharge	1,012 J $^{o}C^{-1}$ kg^{-1} (default)
Molecular weight of discharge	28.96 (default)
Met data	Hourly sequential in 10° sectors Use model default advanced meteorological parameters
Outputs	Annual average
Chemistry module	Off

Run model to provide output files with predicted annual mean concentration at each receptor.

10.4 Area source dispersion model kernel

Prepare 1 km x 1 km dispersion model kernels using ADMS 3. The source-receptor relationship for the central node of the kernel is modified so that emissions within 50 m of a background receptor location are not taken into account: the emissions from a 100 m x 100 m square surrounding the receptor are reallocated throughout the rest of the 1 km x 1 km square (see Figure 6.1).

Parameter	Value
Emission area coordinates, m	{-500,-500} {500,-500} {500, 500} {-500, 500}
Volume source depth	10 m
Emission rate	1 g/s
Receptor area coordinates, m	{-30000,-30000} {30000, 30000}
Surface roughness	1 m
Dry deposition velocity	0
Wet deposition	0
Molecular weight of discharge	28.96 (default)
Met data	Hourly sequential in 10° sectors Use model default advanced meteorological parameters
Outputs	Annual mean
Chemistry module	Off

Run model to provide output kernels. Prepare small industrial source kernel (see Appendix 2).

10.5 Area source modelling

Obtain 1 km x 1 km area source emissions data from NAEI.

Use ArcInfo ’focal sum’ function to multiply each area source emission by the appropriate factor in the dispersion kernel and sum the contributions from each emission source at the centroid of each 1 km x 1 km receptor square.

10.6 Long-range modelling

Prepare 50 km EMEP grid emission input files from EMEP inventory for relevant source sectors.

Obtain 1 km x 1 km gridded oxides of nitrogen, sulphur dioxide and PM_{10} area source data from NAEI. Obtain point source emission data for relevant source sectors from NAEI. Aggregate source data onto 10 km x 10 km grid.

Run TRACK model, Version 1.6f. Version 1.6f assesses the contribution to secondary particulate concentrations from sulphur dioxide and oxides of nitrogen emissions. Also include particulate matter emissions as an inert tracer with dry deposition velocity 0.001 m s^{-1} and wet removal coefficient of 1.3×10^{-5} s^{-1}.

Other input parameters are as follows:

Parameter	**Value**
Receptor grid	Ordnance survey
Receptor square dimension	20 km
Stability class	4
Meanwind speed	7.5 m s^{-1}
Trajectory duration	96 hours
Trajectory timestep	120 seconds
Lookup timestep	2,880 seconds
Number of incoming trajectories at receptor	24
Number of trajectories per 24-hour period	4
Choice of solver	Fixed timestep
Number of vertical levels	Single level
Deposition velocities	Spatially disaggregated values from input file
Choice of season	All year
Seeder-feeder enhancement	On
Seeder-feeder effect cut-in level	800 mm rain per year
Seeder-feeder factor on wet deposition rate	2
Seeder-feeder factor on sulphur dioxide oxidation rate	1.3
Tracer	On
Source type	Area sources

10.7 Model calibration

Particulate sulphate, nitrate and chloride concentrations are measured at 12 sites in the UK Acid Deposition Network. Particulate sulphate consists of components derived from non-marine sources and from seawater. The measurements of particulate chloride concentrations may be used to distinguish between the marine sulphate and non-marine sulphate components following the guidance in the ICP Mapping Manual (http://www.oekodata.com/icpmapping/html/manual.html):

$$[SO_4^{2-}]_{non-marine} = [SO_4^{2-}]_{measured} - 0.103\left[Cl^-\right]_{measured}$$

where the concentrations are in equivalents per litre.

A regression analysis of the non-marine sulphate data may then be carried out of the form:

$$c_{measured} = Ac_{long\_range}$$

where A is determined by the regression analysis.

A similar regression analysis of modelled and measured particulate nitrate should also be carried out.

Identify rural, suburban, urban background and urban centre monitoring sites in Defra's automatic and urban rural network, with the year's ratified data and with more than 75 per cent data capture. Derive annual means. A further regression analysis should then be carried out to determine the coarse particulate contribution.

$$[PM_{10}] = A + rs[SO_4^{2-}]_{Track} + tu[NO_3^-]_{Track} + [PM_{10}]_{Track} + [PM_{10}]_{adms\_area} + [PM_{10}]_{adms\_pts} + [SO_4^{2-}]_{marine}$$

where:

A is a coefficient determined by regression analysis;
r is a mass adjustment factor assuming that all the sulphate is present as ammonium sulphate = 1.354;
t is a mass adjustment factor assuming that all the nitrate is present as ammonium nitrate adjusted further empirically to allow for the volatility of ammonium nitrate in the TEOM measuring device = 1;
s is the calibration factor relating measured and modelled sulphate concentrations = 1.61;
u is the calibration factor relating measured and modelled nitrate concentrations = 0.765;

$[SO_4^{2-}]_{Track}$ is the sulphate concentration modelled using TRACK;
$[NO_3^-]_{Track}$ is the nitrate concentration modelled using TRACK;
$[PM_{10}]_{adms\_area}$ is the contribution from UK one km area sources modelled by ADMS;
$[PM_{10}]_{adms\_pts}$ is the contribution from Environment Agency-regulated large point sources modelled by ADMS;
$[PM_{10}]_{Track}$ is the contribution from long-range primary PM_{10} emissions modelled by TRACK;
$[SO_4^{2-}]_{marine}$ is the marine sulphate concentration determined from the measurement data, typically 0.15 μg m^{-3}.

Obtain the following:

- nearest neighbour prediction from ADMS point source dispersion modelling at each monitoring station, $c_{modelled\_industrial}$
- nearest neighbour prediction from ADMS area source modelling at each monitoring station, $c_{modelled\_area}$
- nearest neighbour prediction from long-range modelling of primary PM_{10} at each monitoring station, $c_{long\text{-}range\_primary}$

Carry out an analysis to obtain calibration factors based on a regression model for PM_{10} of the form:

$$c_{measured} = c_{modelled\_industrial} + B + Ac_{modelled\_area} + c_{long\_range\_primary} + PM_{10\_secondary}$$

where:

- A is a constant determined by the regression analysis;
- B is a constant variously determined by the regression analysis or on the basis of a priori judgement.

The offset B is assumed to be representative of coarse or other particulate sources.

Determine prediction intervals (see Section 3.6.5).

10.8 ArcInfo GIS maps

For each 1 km x 1 km grid square centroid throughout the UK, carry out the following:

Interpolate point source model predictions of percentile concentrations onto one km grid.

Add contributions from area sources, long-range primary and secondary sources and other sources by application of the calibration model.

Convert TEOM-based estimates to gravimetric basis by multiplying by 1.3.

Plot modelled concentrations as a map of the UK.

References and Bibliography

Abbott, J., and Vincent, K., 1999. *Annual average sulphur dioxide concentration maps derived by dispersion modelling*. AEA Technology, National Environmental Technology Centre. Report AEAT - 4629 http://www.aeat.co.uk/netcen/airqual/reports/kvann1/so2ann.html

Abbott, J. and Downing, C, 2000. *The addition of background concentrations to modelled concentrations from discharge stacks*. R&D Technical Report P361 produced for the Environment Agency.

Abbott, J., Hayman, G., Vincent, K.J., Metcalfe, S., Dore, T., Skeffington, R., Whitehead, P., Whyatt, D., Passant, N. and Woodfield, M., 2003. *Uncertainty in acid deposition modelling and critical load assessments*. A report produced for the Environment Agency (available at http://publications.environment-agency.gov.uk/pdf/SP4-083-5-1-e-e.pdf).

Coleman, P., Bush, T., Conolly, C., Irons, S., Murrells, T., Vincent, K.J. and Watterson, J., 2001. *Assessment of benzo[a]pyrene atmospheric concentrations in the UK to support the establishment of a national PAH objective*. A report produced for the Department for Environment, Food and Rural Affairs, the National Assembly for Wales, the Scottish Executive and the Department of the Environment for Northern Ireland. AEAT/ENV/R/0620. Issue 5.1.1.

Hasler, S., Hayman, G.D., Baker, S., Smith, M., Sansom, L. and Page, H., 2001. *Rural Sulphur Dioxide Monitoring in the UK: 1997*. AEA Technology Report AEAT/R/ENV/0040 Issue 2 prepared on the contract TO 7078D1*/Acid Deposition Processes* (EPG 1/3/94). AEA Technology plc, National Environmental Technology Centre. 551 Harwell, OX11 0QJ. Oxfordshire.

Laxen, D. and Wilson, P., 2002. *Compilation of diffusion tube collocation studies carried out by local authorities*. Air Quality Consultants.

Lee, D.S., Kingdon, R.D., Jenkin, M.E. and Garland, J.A., 2000. Modelling the atmospheric oxidised and reduced nitrogen budgets for the UK with a Lagrangian multi-layer long-range transport model. *Environmental Modelling and Assessment*, 5, 83-104.

Stedman, J.R., Bush, T.J., Vincent, K.J. and Baggott, S., 2003. *UK air quality modelling for annual reporting 2002 on ambient air quality assessment under Council Directives 96/62/EC and 1999/30/EC*. AEA Technology, National Environmental Technology Centre. Report AEAT/ENV/R/1564.
http://www.airquality.co.uk/archive/reports/cat05/0402061100_dd12002mapsrep1-2.pdf

List of abbreviations

ADMS	an atmospheric dispersion model
APEG	Airborne Particles Expert Group
AQEG	Air Quality Expert Group
AUN	Automatic Urban Network
BATNEEC	Best Available Technology Not Entailing Excessive Cost
d.f.	degrees of freedom
Defra	Department for Environment, Food and Rural Affairs
EPA	Environmental Protection Act
EPAQS	Expert Panel on Air Quality Standards
HARM	Hull Acid Rain Model
GIS	Geographic Information System
Kerbside	Zero to one metre from the kerb
NAEI	National Atmospheric Emission Inventory
Netcen	National Environmental Technology Centre
NO_2	Nitrogen dioxide
NO_x	Oxides of nitrogen
PM_{10}	Particulate matter with an aerodynamic diameter less than 10 $\mu g\ m^{-3}$
Roadside	One to five metres from the kerb
SD	Standard deviation
SO_2	Sulphur dioxide
TEOM	Tapered element oscillating microbalance
TRACK	Trajectory model with Atmospheric Chemical Kinetics

Appendices

Appendix 1: Emission characteristics of large sulphur dioxide sources

	Source description	Source name	X (m)	Y (m)	Height (m)	Diameter (m)	Temperature / Density (kg m^{-3})	Velocity (m s^{-1}) /Volume flux (m^{3} s^{-1}) /Momentum flux (m^{4} s^{-1}) /Mass flux (kg s^{-1})	Pollutant emission rate (g s^{-1})
PlantID	Authorisation	Site	OS_GRE	OS_GRN	height_m	diameter_m			
44	AA2534	Ferrybridge C	446700	424800	198	10	130	19.40	1300.32
45	AA3301	Fiddlers Ferry	354300	386500	199	13	125	19.00	821.28
51	AA2488	Drax	466400	426400	259	15.83	90	30.02	1401.95
53	AP5803	Indian Queens	194000	59100	46	3	150	15.00	0.80
120	AA2011	Ashington A	430600	590200	114.3	6.07	140	15.24	875.19
121	bl6861	Ashington B	428800	589300	76.5	6.475	35	15.13	78.23
158	bl1100	Holyhead	226500	381000	121	9.807	82	7.87	47.75
322	AA2348	Seal Sands	453400	524000	76	2.3	220	18.00	22.55
367	AI0608	Hope	416900	382200	132	4.5	138	12.95	99.25
372	bl7752	Westbury	388620	152640	122	3.7	165	10.23	40.13
373	AH9499	Northfleet	563600	174400	122	2.79	112	22.30	22.20
374	bl3986	Aberthaw Cement	303400	167500	46	3	150	15.00	42.62
413	AA1996	Baglan Bay	274500	192100	162	3.7	190	11.81	15.44
425	af8050	Coryton A	574400	182300	106.7	2.43	160	19.10	22.45
425	af8050	Coryton B	574400	182300	106.7	2.43	160	19.10	31.28
425	af8050	Coryton C	574400	182300	45.7	2.43	182	7.69	13.43
425	af8050	Coryton D	574400	182300	45.7	2.43	182	7.69	13.43
425	af8050	Coryton E	574400	182300	91.4	4.1	254	9.30	40.11
425	af8050	Coryton F	574400	182300	51.8	1.6	277	7.31	6.26
425	af8050	Coryton G	574400	182300	117	2.9	203	11.64	27.79
425	af8050	Coryton H	574400	182300	80.2	4.05	160	4.87	25.03
447	AS7396	Avonmouth A	352600	179100	91.5	2.2	75	12.00	

	Source description	Source name	X (m)	Y (m)	Height (m)	Diameter (m)	Temperature / Density (kg m^{-3})	Velocity (m s^{-1}) /Volume flux (m^3 s^{-1}) /Momentum flux (m^4 s^{-1}) /Mass flux (kg s^{-1})	Pollutant emission rate (g s^{-1})
458	AA2470	Eggborough	457500	424500	198	12	130	27.00	1648.40
495	AA3093	Cantley	638600	303400	46	3	150	15.00	15.91
534	bk9504	Tunstead	410000	374500	40	3	150	15.00	15.63
537	AF8343	South Wirral	341500	375900	46	3	150	15.00	43.60
564	bl7272	Clitheroe	375200	443700	104.5	4.2	220	12.67	93.79
565	Al0349	Padeswood	329100	362400	41	2.4	150	15.00	110.33
709	AF8173	SouthKillingholmeA	516100	416500	92	4.23	520	9.04	28.96
709	AF8173	SouthKillingholmeB	516100	416500	64	1.67	475	17.00	20.51
709	AF8173	SouthKillingholmeC	516100	416500	115	2.8	272	18.78	10.34
709	AF8173	SouthKillingholmeD	516100	416500	92	2.44	605	21.70	19.31
709	AF8173	SouthKillingholmeE	516100	416500	122	5.94	570	18.70	93.43
741	AA2216	Scunthorpe B	492000	409500	96	3.8	200	14.81	14.72
741	AA2216	Scunthorpe C	492000	409500	76.5	4.24	176	17.19	12.39
742	AF7193	Scunthorpe D	492000	409500	76	3.75	300	5.00	58.66
744	AR0080	Scunthorpe E	492000	409500	107	6.4	160	15.45	74.52
744	AR0080	Scunthorpe F	492000	409500	107	6.4	160	15.45	74.52
751	AA2950	Redcar A	456730	525690	115.5	3.02	200	20.50	0.00
754	AF8530	South Bank	453890	521500	88.4	4.27	250	4.00	28.73
755	af8548	Redcar B	456290	525880	88.7	4.24	260	15.20	53.49
755	af8548-nh3inc	Redcar C	456290	525880	120	1.98	293	10.10	70.91
757	AF8866	Redcar D	457700	524200	0	0	0	0.00	0.00
757	AF8866	Redcar E	457700	524200	0	0	0	0.00	0.00
757	AF8866	Redcar F	457700	524200	0	0	0	0.00	0.00
757	AF8866	Redcar G	457700	524200	0	0	0	0.00	0.00
759	ar0241 -a2	Redcar H	457700	524200	105	6.2	134	12.70	62.01
759	ar0241 -a5	Redcar I	457700	524200	70	6.48	225	5.00	4.80
759	ar0241 ps	Redcar J	457700	524200	115.3	5.23	200	12.10	15.21

	Source description	Source name	X (m)	Y (m)	Height (m)	Diameter (m)	Temperature / Density (kg m^{-3})	Velocity (m s^{-1}) /Volume flux (m^3 s^{-1}) /Momentum flux (m^4 s^{-1}) /Mass flux (kg s^{-1})	Pollutant emission rate (g s^{-1})
759	ar0241reheat	Redcar K	457700	524200	70	2.5	270	20.30	8.38
760	AF8238	Rotherham	444800	395100	65	3	150	15.00	0.00
770	AA2631	Llanwern A	336900	186700	82.3	2.97	164	18.50	0.00
770	AA2631	Llanwern B	336900	186700	51.8	2.59	183	25.70	0.00
777	AA2780	Port Talbot A	278200	187000	121	3.89	200	10.77	13.15
777	AA2780	Port Talbot B	278200	187000	37	2.7	210	7.16	13.15
778	AF8645	Morfa	277900	187100	127	4.7	230	4.50	22.07
781	AR0357	Port Talbot C	278200	187000	74	4.95	190	9.57	106.16
781	AR0357	Port Talbot D	278200	187000	133	8.35	123	7.25	106.16
784	AA3433	Cottam	481700	379700	198	15.8	125	18.00	2787.29
964	AF7886	Milford Haven A	188600	208700	110	4	276	18.30	57.85
964	AF7886	Milford Haven B	188600	208700	100	1.6	250	8.31	3.62
964	AF7886	Milford Haven C	188600	208700	110	4.24	230	8.83	59.06
986	AA3069	Wilton A	456910	521970	0	0	0	0.00	0.00
986	aa3069-4	Wilton B	456910	521970	137	4.88	120	12.08	200.31
986	AA3069	Wilton C	456910	521970	0	0	0	0.00	0.00
986	AA3069	Wilton D	456910	521970	0	0	0	0.00	0.00
996	AF8009	Fawley A	444300	103800	107	3	200	15.00	81.66
996	AF8009	Fawley B	444300	103800	73	3	200	15.00	83.91
996	AF8009	Fawley C	444300	103800	137	3	200	15.00	93.84
996	AF8009	Fawley D	444300	103800	37	3	200	15.00	48.72
996	AF8009	Fawley E	444300	103800	62	3	200	15.00	92.48
996	AF8009	Fawley F	444300	103800	63	3	200	15.00	50.53
1189	AH9464	Stewartby	501700	242600	70	2.4	108	9.00	271.56
1192	AH6554	Kings Dyke	524400	297700	53	3	150	15.00	121.45
1292	af8319-stack1	Middlesborough A	452690	523320	104	4.27	235	3.81	38.05
1292	af8319-stack2	Middlesborough B	452690	523320	114	4.57	316	2.65	38.05

	Source description	Source name	X (m)	Y (m)	Height (m)	Diameter (m)	Temperature / Density (kg m^{-3})	Velocity (m s^{-1}) /Volume flux (m^3 s^{-1}) /Momentum flux (m^4 s^{-1}) /Mass flux (kg s^{-1})	Pollutant emission rate (g s^{-1})
1394	AA3204	Tilbury B	566200	175600	171	6.3	140	19.06	504.19
1402	AA3115	Fawley	447400	102300	198	17	150	21.30	15.79
1403	AA3166	Littlebrook D	555800	176500	215	11.3	140	31.00	20.90
1404	AA3107	Didcot A	451300	191900	198	12	150	20.55	1331.81
1407	AA2682	Aberthaw B	302300	166000	152	6.8	126	23.40	1178.92
1525	AI0438	Whitwell	454000	374700	96	4	150	15.00	72.11
1526	AI0179	Thrislington	430800	532800	76	3	150	15.00	
1573	AF6928	Killingholme A	515800	417700	98	4.1	230	10.50	75.20
1573	AF6928	Killingholme B	515800	417700	91	2.7	350	17.50	37.43
1573	AF6928	Killingholme C	515800	417700	137	4.7	245	12.50	150.73
1573	AF6928	Killingholme D	515800	417700	132	3.99	205	10.56	70.85
1671	AF7835	Barnsley	437600	412200	45	1.83	150	15.00	
1810	AF7215	NorthTees A	452960	523080	49	2.5	240	5.79	8.45
1810	AF7215	NorthTees B	452960	523080	61	2.44	160	2.55	4.89
1810	AF7215	North Tees C	452960	523080	40	1.32	420	9.74	31.12
1868	AA2267	Ratcliffe on Soar	450400	329700	199	11.9	80	23.50	781.08
1870	AA3000	Kingsnorth	580600	172200	198	12.2	130	26.00	1327.37
1977	AL9459	Chesterfield	442100	374900	85.3	4.18	150	15.00	11.65
2076	AA2658	Rugeley B	405900	317100	183	8.8	130	23.00	1241.15
2145	AF7916	Avonmouth B	353470	181630	46	2.01	223	26.50	73.68
2165	AF8394	Stanlow A	343800	375800	75	2.6	225	4.80	13.83
2165	AF8394	Stanlow B	343800	375800	125	1	280	4.40	38.02
2165	AF8394	Stanlow C	343800	375800	122	5	230	4.60	17.28
2165	AF8394	Stanlow D	343800	375800	155	7.45	175	10.10	145.17
2165	AF8394	Stanlow E	343800	375800	80	3.5	160	13.10	114.06
2165	AF8394	Stanlow F	343800	375800	143	4	175	4.40	17.28
2339	AF7894	Pembroke A	191000	202300	162	2.97	160	8.79	27.26

	Source description	Source name	X (m)	Y (m)	Height (m)	Diameter (m)	Temperature / Density (kg m^{-3})	Velocity (m s^{-1}) /Volume flux (m^{3} s^{-1}) /Momentum flux (m^{4} s^{-1}) /Mass flux (kg s^{-1})	Pollutant emission rate (g s^{-1})
2339	AF7894	Pembroke B	191000	202300	167	4.38	230	6.16	41.67
2339	AF7894	Pembroke C	191000	202300	92	3.3	180	7.83	29.92
2339	AF7894	Pembroke D	191000	202300	92	2.7	180	14.50	37.24
2339	AF7894	Pembroke E	191000	202300	158	3.95	156	15.61	85.56
2421	AA3212	West Burton	479100	385700	183	8.9	125	25.00	2584.35
2422	AA2674	Ironbridge	365400	303800	204	8.58	130	27.60	1147.89
2423	AA2925	Drakelow C	424000	319500	168	8.1	144	10.40	159.82
2424	AA3425	High Marnham	485700	370600	137	11.7	132	16.00	192.16
2428	AO2353	Bridgwater	331100	138000	53	3	150	15.00	57.05
2590	0087/99A	Cookstown	89567	539888	40	3	150	15.00	22.64
2591	IPC/E/00016	Dunbar	370240	675640	40	3	150	15.00	178.53
2597	IPC/N/50007	Lochaber	212630	775039	30	2.1	80	16.80	24.80
2601	IPC/E/00039	Cockenzie	340000	675000	149	7.35	132	22.00	726.15
2602	IPC/E/00069	Longannet	300000	687000	183	15.12	110	18.60	1699.64
2604	0010/98A	Belfast West A	145500	531000	73	3.66	140	15.00	0.00
2604	0010/98A	Belfast West B	145500	531000	198	12	150	20.00	0.00
2604	0010/98A	Belfast West C	145500	531000	73	3.96	140	15.00	0.00
2605	0011/98A	Kilroot A	154500	541000	198	12	150	20.00	206.32
2605	0011/98A	Kilroot B	154500	541000	200	5.5	120	17.64	230.80
2606	0007/98A	Coolkeeragh A	62000	584500	81	3.8	150	15.00	8.82
2606	0007/98A	Coolkeeragh B	62000	584500	81	4.42	150	15.00	11.93
2606	0007/98A	Coolkeeragh C	62000	584500	81	3.8	150	15.00	8.82
2606	0007/98A	Coolkeeragh D	62000	584500	198	12	150	20.00	15.29
2607	0008/98A	Ballylumford A	157900	558000	124	5.9	140	15.00	1.57
2607	0008/98A	Ballylumford B	157900	558000	124	5.9	140	15.00	1.57
2607	0008/98A	Ballylumford C	157900	558000	124	5.9	140	15.00	1.57
2607	0008/98A	Ballylumford D	157900	558000	198	12	150	20.00	36.55
2608	IPC/N/20019	Peterhead	412000	845000	165	9.4	145	20.00	2.38

	Source description	Source name	X (m)	Y (m)	Height (m)	Diameter (m)	Temperature / Density (kg m^{-3})	Velocity (m s^{-1}) /Volume flux (m^3 s^{-1}) /Momentum flux (m^4 s^{-1}) /Mass flux (kg s^{-1})	Pollutant emission rate (g s^{-1})
3081	IPC/E/00011	Grangemouth	294351	680627	100	3	150	15.00	101.79
3145	IPC/E/00060	Glenrothes	327900	701400	32	1.7	150	15.00	28.54
3319	0143/01A	Maydown A	66000	584200	73	1.3	140	15.00	10.94
3319	0143/01A	Maydown B	66000	584200	73	1.3	140	15.00	2.45
3319	0143/01A	Maydown C	66000	584200	73	1.3	140	15.00	4.93
3319	0143/01A	Maydown D	66000	584200	73	1.3	140	15.00	2.45
4384	BK6629	Oughtibridge	430200	394100	46	3	150	15.00	5.24
4402	BL1029	South Ferriby	497300	420900	53	3	150	15.00	32.98

Appendix 2: Small point source model

Introduction

Small industrial sources have generally been represented in earlier maps (Stedman *et al.*, 2002) as one km square volume sources. However, this approach has in some cases led to unreasonably high concentrations close to the source. The overestimation arises because the release height, buoyancy and momentum of discharges from industrial chimneys is not taken into account. A revised small point source model has been developed which uses dispersion kernels that will take these factors into account.

The dispersion model ADMS 3.1 was used to prepare the dispersion kernels.

Discharge conditions

The National Atmospheric Emission Inventory contains limited information on the discharge characteristics of individual emission sources. In many cases, the information is limited to data on the total annual emission of individual pollutants. It is therefore necessary to make some general assumptions about the discharge height, discharge temperature, volumetric flow rate of the discharge and the discharge velocity. Our approach has been to make reasonable but generally conservative assumptions corresponding to industrial practice.

Sulphur dioxide

For sulphur dioxide, it was assumed that the plant operates continuously throughout the year. The stack height was estimated using the following equations taken from the 3rd edition of the Chimney Heights Memorandum:

If the sulphur dioxide emission rate, R_A (kg/h), is less than 10 kg/h, the chimney height, U (m), is given by:

$$U = 6R_A^{0.5}$$

If R_A is in the range 10-100 kg/h:

$$U = 12R_A^{0.2}$$

Emission rates in excess of 100 kg/h were not considered in this study.

No account was taken of the effects of buildings: it was assumed that the increase in chimney height to take account of building effects provided by the Memorandum would compensate for the building effects.

It was then assumed that the sulphur dioxide concentration in the discharge would be at the limit for indigenous coal and liquid fuel for new and existing plant provided by Secretary of State's Guidance-Boilers and Furnaces, 20-50 MW net rated thermal input PG1/3(95). The limit is 3,000 mg m^{-3} at reference conditions of 273 K, 101.3 kPa, six per cent oxygen for solid fuel firing and three per cent oxygen for liquid firing and dry gas. It was assumed that the oxygen content in the discharge corresponded with the reference condition. The moisture content of the discharge was ignored. It was assumed that the temperature of discharge was 373 K: higher temperatures would lead to improved buoyancy and hence lower ground level concentrations, while lower temperatures would usually result in unacceptable water condensation. A discharge velocity of 10 m/s was selected to be representative of most combustion source discharges. The discharge diameter d (m) was calculated from:

$$d = \sqrt{\frac{4qT}{273\pi cv}}$$

where q is the sulphur dioxide emission rate, g/s
T is the discharge temperature, 373 K
c is the emission concentration at reference conditions, 3 g m^{-3}
v is the discharge velocity, 10 m/s

Table A2.1 shows the modelled stack heights and diameters.

Table A2.1: Modelled stack heights and diameters for sulphur dioxide

Emission rate			Stack height, m	Stack diameter, m
g/s	kg/h	t/a		
0.1	0.36	3.2	3.60	0.08
0.2	0.72	6.3	5.09	0.11
0.5	1.8	15.8	8.05	0.17
1	3.6	31.5	11.38	0.24
2	7.2	63.1	16.10	0.34
5	18	157.7	21.39	0.54
10	36	315.4	24.57	0.76
20	72	630.7	28.23	1.08

Oxides of nitrogen

For nitrogen dioxide, it was assumed that the plant operates continuously throughout the year. The stack height was estimated using the following equation taken from the 3rd edition of the Chimney Heights Memorandum for very low sulphur fuels:

$$U = 1.36Q^{0.6}\left(1 - 4.7 \times 10^{-5} Q^{1.69}\right)$$

where Q is the gross heat input in MW.

This relationship applies for heat inputs up to 150 MW. For larger heat inputs, a fixed height of 30 m was used corresponding to an approximate lower limit derived from available data on stack heights for large sources.

The gross heat input used in the above equation was calculated from the oxides of nitrogen emission rate, using an emission factor of 10,600 kg/MTh (0.100 g/MJ) for oxides of nitrogen emitted from natural gas combustion in non-domestic non-power station sources taken from the NAEI.

For fuels containing significant sulphur, the actual stack height will be greater to allow for the dispersion of sulphur dioxide and this is expected to lead to an overestimate of ground level concentrations.

The emission limits for oxides of nitrogen provided by Secretary of States Guidance-Boilers and Furnaces, 20-50 MW net rated thermal input PG1/3(95), depend on the type of fuel and are in the range 140-650 mg m^{-3} at reference conditions. A value of 300 mg m^{-3} was used in the calculation of the stack discharge diameter. Other assumptions concerning discharge conditions followed those made for sulphur dioxide above.

Table A2.2 shows the modelled stack heights and diameters.

Table A2.2: Modelled stack heights and diameters for oxides of nitrogen

Emission rate g/s	t/a	Height, m	Diameter, m
0.1	3.2	1.36	0.24
0.2	6.3	2.06	0.34
0.5	15.8	3.57	0.54
1	31.5	5.40	0.76
2	63.1	8.15	1.08
5	157.7	13.72	1.70
10	315.4	19.12	2.41
20	630.7	21.34	3.41
50	1576.8	30.00	5.38
100	3153.6	30.00	7.61

Particulate matter, PM_{10}

The stack heights and diameters used for oxides of nitrogen were also used to provide the kernels for particulate matter PM_{10}. This provides a conservative assessment of PM_{10} concentrations for the following reasons. The emission limits for total particulate matter provided by Secretary of State's Guidance-Boilers and Furnaces, 20-50 MW net rated thermal input PG1/3(95), depend on the type of fuel and are in the range 5-300 mg m^{-3} at reference conditions. The emission limit for total particulate matter includes, but is not limited to, the contribution from PM_{10}.

Dispersion modelling

The dispersion model ADMS 3.1 was used to predict ground level concentrations on two receptor grids:

- an in-square grid covering an area 1 km x 1 km with the source at the centre and with receptors at 33.3 m intervals;
- an outer-grid covering an area 30 km x 30 km with the source at the centre and with receptors at one km intervals.

A surface roughness value of 0.5 m was used, corresponding to areas of open suburbia. Meteorological data for Heathrow for the years 1993-2002 was used in the assessment, with most model runs using the 2000 data.

Results

Sulphur dioxide

Table A2.3 shows the predicted in-square average concentration for the one km square centred on the emission source for 2000 meteorological data.

Table A2.3: Predicted in-square concentration for sulphur dioxide

Emission rate, g/s	Average in square concentration, $\mu g\ m^{-3}$
0.1	0.599
0.2	0.934
0.5	1.555
1	2.19
2	2.92
5	4.57
10	6.56
20	8.86

The results shown in Table A2.3 may be approximated by the relationship:

$$C=Aq^{0.5}$$

where C is the in-square concentration, $\mu g\ m^{-3}$, and q is the emission rate, g/s. A is a proportionality factor (2.07 in 2000)

Table A2.4 shows the predicted in-square concentration for an emission rate of 10 g/s for meteorological years 1993-2002. Table A2.4 also shows the inter-annual variation in the factor A.

Table A2.4: In-square concentrations for 10 g/s emissions

Year	In-square concentration, $\mu g\ m^{-3}$	Factor A
1993	6.21	1.96
1994	6.01	1.90
1995	6.12	1.94
1996	6.23	1.97
1997	6.10	1.93
1998	6.18	1.95
1999	6.49	2.05
2000	6.56	2.07
2001	6.32	2.00
2002	6.51	2.06

Figure A2.1 shows the predicted outer-grid concentration along the east-west axis through the source for 2000 meteorological data for a range of rates of emission (in g/s). Figure A2.1 does not include results for the one km source square.

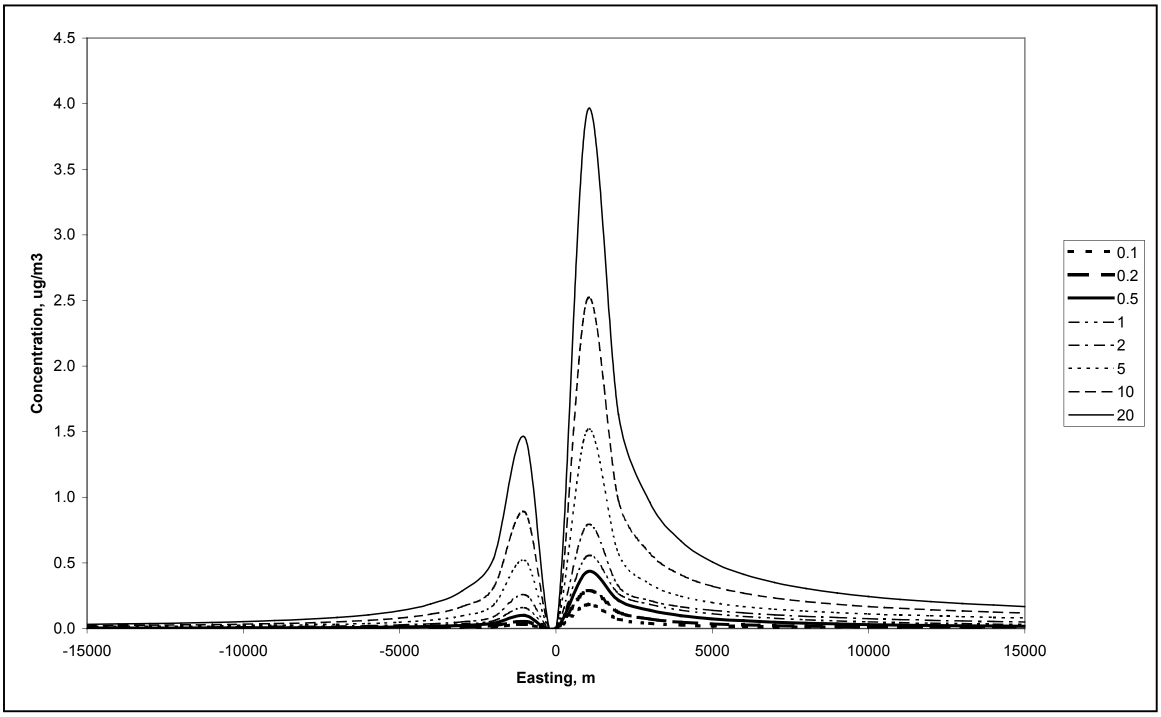


Figure A2.1: Sulphur dioxide concentration on east-west axis, 2000 meteorological data

Figure A2.2 shows the same model results plotted as $C/q^{2/3}$. The spread of the model results is greatly reduced so that as a reasonable approximation, all the model results may be reduced to a single line.

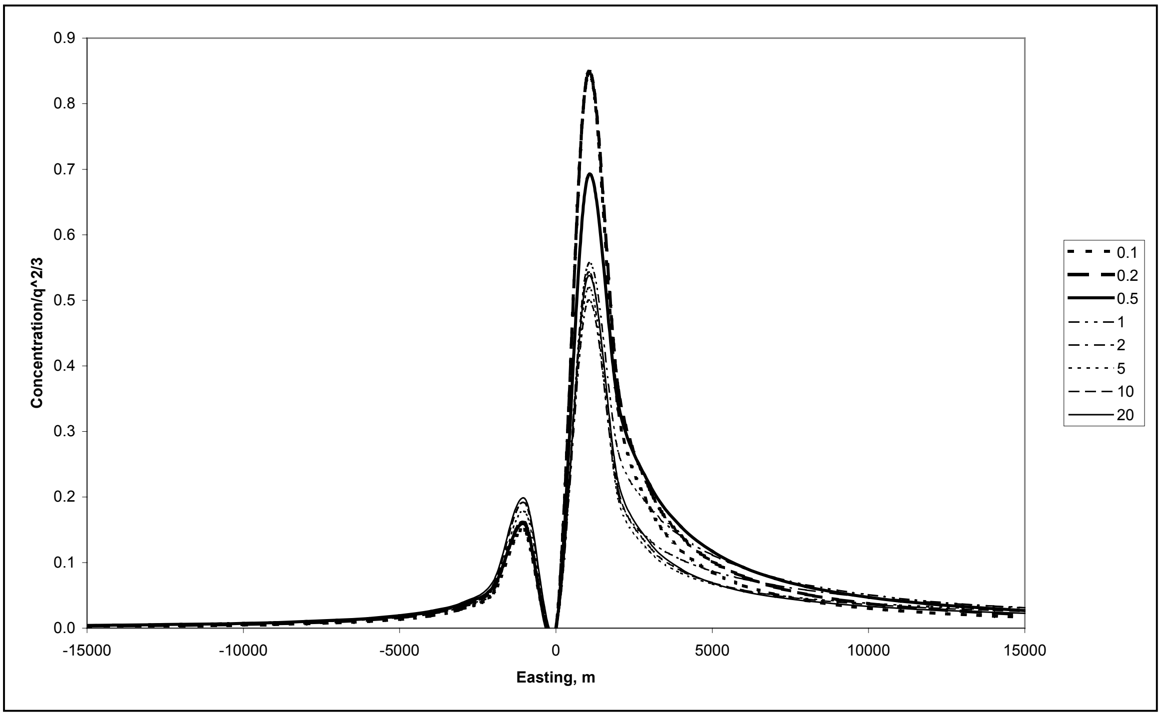


Figure A2.2: Reduced sulphur dioxide concentrations on the east-west axis, 2000 meteorological data

Thus, the results for an emission rate of 10 g/s were used for all emission rates in the range 0.1-20 g/s in the preparation of dispersion kernels for industrial sulphur dioxide emissions. The dispersion kernel was multiplied by $10(q/10)^{2/3}$ to provide estimates of the impact of emission q (g/s) at each receptor location. Separate kernels were created from each meteorological data year 1993-2002.

Oxides of nitrogen

Table A2.5 shows the predicted in-square average concentration for the one km square centred on the emission source for 2000 meteorological data.

Table A2.5: In-square oxides of nitrogen concentrations, 2000

Emission rate, g/s	In square concentration, $\mu g\ m^{-3}$
0.1	0.464
0.2	0.764
0.5	1.37
1	1.97
2	2.6
5	3.31
10	3.58
20	4.34
50	3.745
100	4.3

The results shown in Table A2.5 may be approximated in the range 0.1-20 g/s by the relationship:

$$C=B\ \log_{10}(10q)+0.464$$

where C is the in-square concentration, $\mu g\ m^{-3}$, q is the emission rate, g s^{-1}, and B is a numerical constant, 1.68 in 2000.

For emission rates in the range 20-100 g s^{-1}, the in-square concentration is approximately 4 $\mu g\ m^{-3}$.

Table A2.6 shows the predicted in-square concentration for an emission rate of 20 g s^{-1} for meteorological years 1993-2002. Table A2.6 also shows the inter-annual variation in the factor B.

Table A2.6: Inter-annual variation in in-square oxides of nitrogen concentration

Year	In-square concentration, $\mu g\ m^{-3}$	Factor B
1993	3.62	1.37
1994	3.88	1.48
1995	3.74	1.42
1996	4.3	1.67
1997	3.66	1.39
1998	3.64	1.38
1999	4.14	1.60
2000	4.34	1.68
2001	4.02	1.55
2002	4.68	1.83

Figure A2.3 shows the predicted outer-grid oxides of nitrogen concentration along the east-west axis through the source for a range of rates of emission (in g s^{-1}).

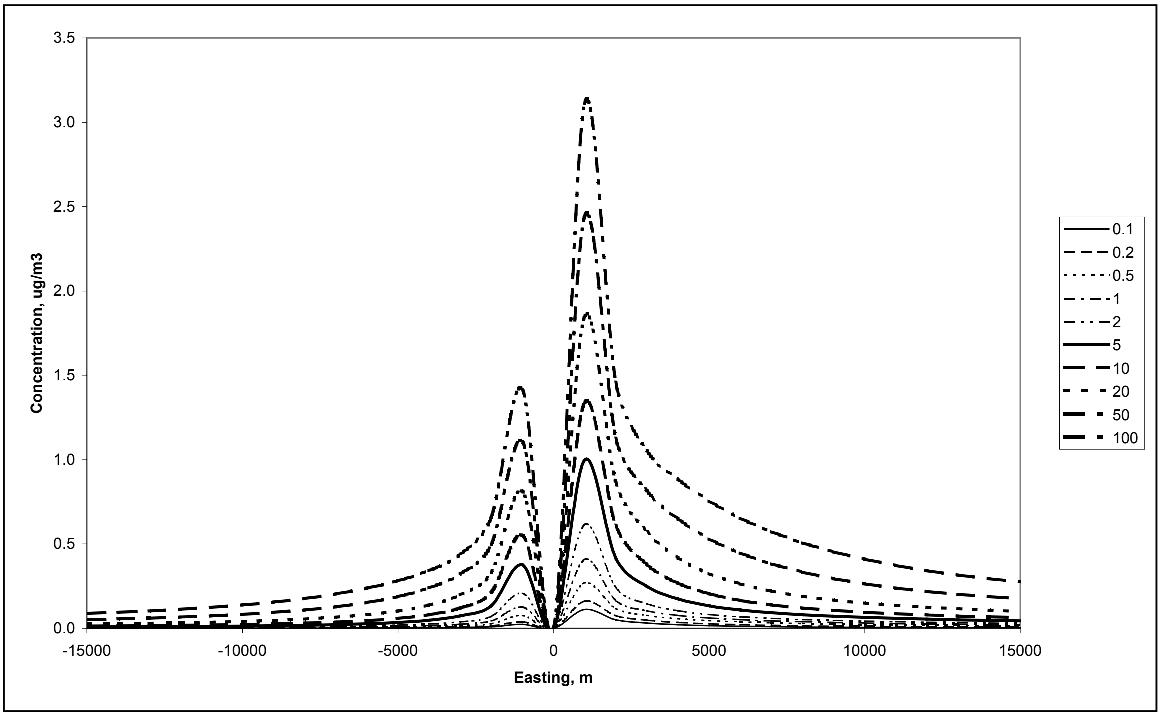


Figure A2.3: Oxides of nitrogen concentration on east-west axis, 2000 meteorological data

Figure A2.4 shows the same model results plotted as $C/q^{0.6}$. The spread of the model results is greatly reduced so that as a reasonable approximation, all the model results may be reduced to a single line.

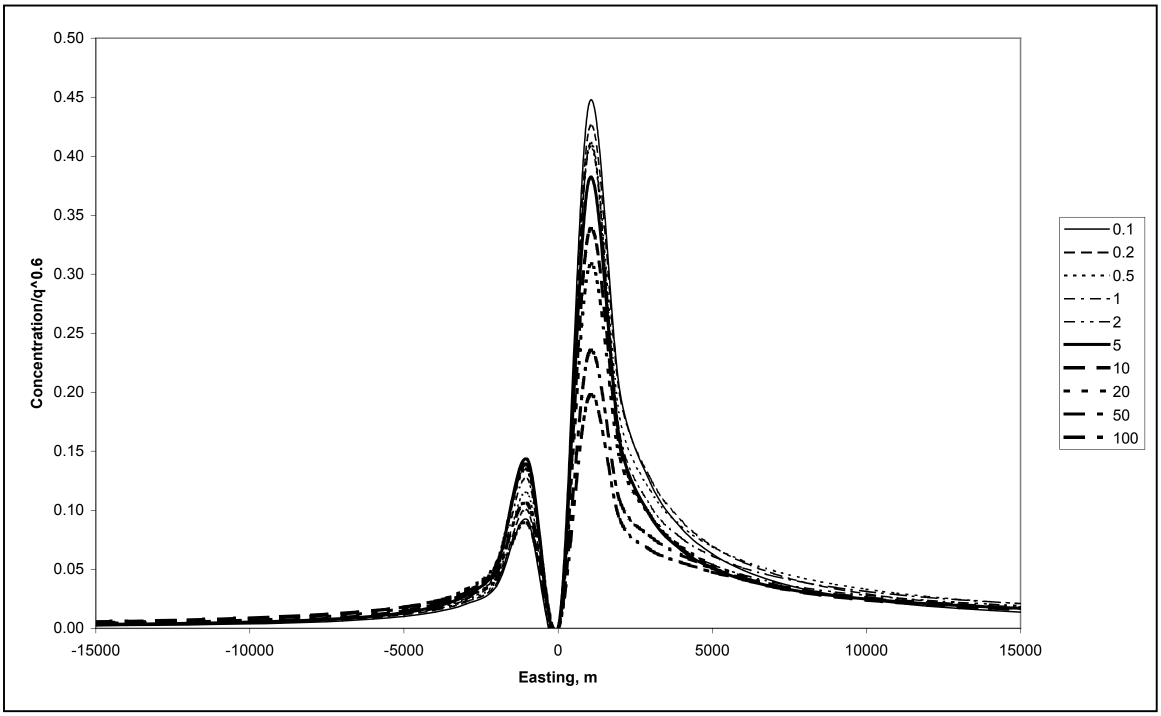


Figure A2.4: Reduced oxides of nitrogen concentrations on the east-west axis, 2000 meteorological data

Thus, the results for an emission rate of 20 g/s were used for all emission rates in the range 0.1-100 g/s in the preparation of dispersion kernels for oxides of nitrogen emissions. The dispersion kernel was multiplied by $20(q/20)^{0.6}$ to provide estimates of the impact of emission q (g/s) at each receptor location. Separate kernels were created for each meteorological data year 1993-2002.

Method

Sulphur dioxide

Point sources with emissions greater than or equal to 500 tonnes per year (15.85 g/s) were modelled explicitly using ADMS. Point sources with emissions less than 500 tonnes per year were modelled using the small points model. This model has two components.

The in-square concentration for each source was calculated using the following function:

$$C=1.98q^{0.5}$$

where C is the in-square concentration, $\mu g\ m^{-3}$, q is the emission rate, $g\ s^{-1}$, and 1.98 is a numerical constant, calculated as the average value over the years 1993-2002 for meteorological data at Heathrow.

The outer-grid concentration was calculated by adjusting the emissions for each source using the function:

$$Q = 10(q/10)^{0.667}$$

where q is the emission rate, g/s, and Q is the adjusted emissions. The sum of the adjusted emission was then calculated for each grid square and the outer-grid concentration calculated using a small points dispersion kernel (which was calculated as the average over the years 1993-2002 for meteorological data at Heathrow).

The in-square and outer-grid concentrations were then summed to calculate the total contribution to ambient annual mean concentrations from these small point sources.

Oxides of nitrogen

Point sources with emissions greater than or equal to 500 tonnes per year (15.85 g/s) were modelled explicitly using ADMS. Point sources with emissions less than 500 tonnes per year were modelled using the small points model. This model has two components.

The in-square concentration for each source was calculated using the following function:

$$C=1.54\log_{10}(10q)+0.464$$

where C is the in-square concentration, $\mu g\ m^{-3}$, q is the emission rate, g/s, and 1.54 is a numerical constant, calculated as the average value over the years 1993-2002 for meteorological data at Heathrow.

The outer-grid concentration was calculated by adjusting the emissions for each source using the function:

$$Q = 20(q/20)^{0.6}$$

where q is the emission rate, g/s, and Q is the adjusted emissions. The sum of the adjusted emission was then calculated for each grid square and the outer-grid concentration calculated using a small points dispersion kernel (which was calculated as the average over the years 1993-2002 for meteorological data at Heathrow).

The in-square and outer-grid concentrations were then summed to calculate the total contribution to ambient annual mean concentrations from these small point sources.

PM_{10}

The method for PM_{10} was the same as for NO_x, except that point sources with emissions greater than or equal to 200 tonnes per year (6.34 g s^{-1}) were modelled using ADMS. Point sources with emissions less than 200 tonnes per year were modelled using the small points model.

Appendix 3: Monitoring stations used in the calibration of the sulphur dioxide model

Site	Site type	East	North
Birmingham Airport	Contract Site	417960	283999
Carrickfergus Rosebrook Avenue	Contract Site	154608	543022
Derry Brandywell	Contract Site	59117	580233
Lisburn Island Civic Centre	Contract Site	138888	520363
Newry Monaghan Row	Contract Site	116267	484684
Newry Trevor Hill	Contract Site	117103	484491
North Down Bangor	Contract Site	162731	535152
Oldham West Endhouse	Contract Site	391870	405513
Ribble Valley Lillands	Contract Site	373650	443650
Salford M60	Contract Site	374813	400853
Strabane Springhill Park	Contract Site	49730	561049
Bexleyheath	Innogy	548300	174500
Didcot South	Innogy	448500	188400
Downes Ground Farm	Innogy	470400	424900
East Tilbury	Innogy	567500	177200
Font-y-gary	Innogy	305300	166100
Hemingbrough	Innogy	466900	429700
North Featherstone	Innogy	442700	422700
Northfleet	Innogy	562600	174700
Smeathalls Fm	Innogy	451200	425200
West Bank	Innogy	462400	425000
West Thurrock	Innogy	559000	176800
London Marylebone Road	KERBSIDE	528100	182000
Bentley Hall Farm	PG	408500	318900
Bottesford	PG	479700	337600
Gainsborough Cemetery	PG	481900	390600
Gillingham	PG	578400	169300
Grove Reservoir	PG	474150	380400
Marton School	PG	484400	381850
Ruddington	PG	456400	332100
Stile Cop Cemetery	PG	403900	316000
Telford Aqueduct	PG	369000	305800
Telford School	PG	368200	304000
Thorney	PG	485800	373100
Weston on Trent	PG	440800	327800
Bury Roadside	ROADSIDE	380922	404772
Exeter Roadside	ROADSIDE	291940	92900
London Cromwell Road 2	ROADSIDE	526523	178947
Newham Cam Road	ROADSIDE	538661	183969
Oxford Centre	ROADSIDE	451366	206152
Southwark Roadside	ROADSIDE	534600	177800
Wrexham	ROADSIDE	332862	349904

Site	Site type	East	North
Bacton Gas Terminal	RURAL	633400	333600
Harwell	RURAL	447400	186300
Ladybower	RURAL	416400	389200
Lullington Heath	RURAL	553800	101600
Rochester	RURAL	583100	176200
V Glamorgan Fonmon	RURAL	305910	167340
Wicken Fen	RURAL	556400	269200
Appleacre	Rural SO2	366500	520800
Barcombe Mills	Rural SO2	543700	114900
Bentra	Rural SO2	158700	545900
Bush	Rural SO2	324600	663800
Bylchau	Rural SO2	295900	359600
Caenby 1	Rural SO2	499300	390000
Camborne 1	Rural SO2	162800	40700
Camphill 1	Rural SO2	227400	654600
Church Fenton	Rural SO2	452800	432800
Corpach 1	Rural SO2	205400	778200
Crai	Rural SO2	286100	218300
Cresselly 1	Rural SO2	206400	206200
Cwmystwyth	Rural SO2	277400	274500
Drayton	Rural SO2	416400	259400
Eskdalemuir	Rural SO2	323500	603000
Etton 1	Rural SO2	498000	444500
Fairseat	Rural SO2	562200	161500
Formoyle	Rural SO2	93900	589300
Forsinain	Rural SO2	290600	948600
Fort Augustus 2	Rural SO2	236600	809100
Garrary	Rural SO2	253100	579000
Glen Dye	Rural SO2	364200	786400
Hebden Bridge 2	Rural SO2	401100	432700
High Muffles	Rural SO2	477600	493900
Husborne Crawley 1	Rural SO2	496400	236100
Little Horkesley 1	Rural SO2	597100	231200
Loch Leven 2	Rural SO2	315900	699000
Marshfield 1	Rural SO2	325500	183000
Pitlochry	Rural SO2	291800	759900
Preston Montford 2	Rural SO2	343200	314300
Redesdale 2	Rural SO2	383300	596100
Rockbourne 1	Rural SO2	411600	118100
Rosemaund	Rural SO2	356400	247600
Stoke Ferry	Rural SO2	570000	298800
Strathvaich Dam	Rural SO2	234700	875000
Sutton Bonington	Rural SO2	450500	326800
Wakefield 24	Rural SO2	435200	413200
Waunfawr 1	Rural SO2	253300	360700
Yarner Wood	Rural SO2	278600	78900
London Bexley	SUBURBAN	551800	176300
London Eltham	SUBURBAN	544000	174700
London Hillingdon	SUBURBAN	506939	178621
Manchester South	SUBURBAN	383912	385828
Redcar	SUBURBAN	459975	524563
Aberdeen	URBAN BACKGROUND	394416	807408

Site	Site type	East	North
Abingdon	URBAN BACKGROUND	449910	197100
Ards	URBAN BACKGROUND	161298	528389
Barnsley 12	URBAN BACKGROUND	434200	406700
Barnsley Gawber	URBAN BACKGROUND	432529	407472
Belfast East	URBAN BACKGROUND	148000	529300
Birmingham East	URBAN BACKGROUND	411536	288870
Bolton	URBAN BACKGROUND	371000	408500
Bournemouth	URBAN BACKGROUND	412300	93344
Castlereagh Espie Way	URBAN BACKGROUND	149800	528200
Coventry Memorial Park	URBAN BACKGROUND	432600	279600
Cwmbran	URBAN BACKGROUND	330510	195436
Derry	URBAN BACKGROUND	60143	581004
Leamington Spa	URBAN BACKGROUND	432060	265906
London Brent	URBAN BACKGROUND	520090	189252
London N. Kensington	URBAN BACKGROUND	524000	181700
London Teddington	URBAN BACKGROUND	515600	170600
Northampton	URBAN BACKGROUND	476111	264524
Port Talbot	URBAN BACKGROUND	278036	188249
Portsmouth	URBAN BACKGROUND	465686	103607
Preston	URBAN BACKGROUND	355200	430100
Sandwell West Bromwich	URBAN BACKGROUND	400300	291500
Southend-on-Sea	URBAN BACKGROUND	585566	186130
Stockport Shaw Heath	URBAN BACKGROUND	389386	389604
Sunderland	URBAN BACKGROUND	439800	557000
Tameside Two Trees School	URBAN BACKGROUND	393440	394377
Thurrock	URBAN BACKGROUND	561018	177894
Trafford	URBAN BACKGROUND	378768	394646
Wigan Leigh	URBAN BACKGROUND	366468	399842
Wirral Tranmere	URBAN BACKGROUND	332096	386644
Belfast Centre	URBAN CENTRE	146231	529911
Birmingham Centre	URBAN CENTRE	406342	286862
Bradford Centre	URBAN CENTRE	416663	433053
Bristol Centre	URBAN CENTRE	359404	173344
Cardiff Centre	URBAN CENTRE	318412	176530
Glasgow Centre	URBAN CENTRE	258902	665028
Hull Freetown	URBAN CENTRE	509400	429300
Leeds Centre	URBAN CENTRE	429976	434268
Leicester Centre	URBAN CENTRE	458768	304820
London Bloomsbury	URBAN CENTRE	530134	181986
London Lewisham	URBAN CENTRE	537700	173800
London Southwark	URBAN CENTRE	532400	178500
Manchester Piccadilly	URBAN CENTRE	384334	398326
Newcastle Centre	URBAN CENTRE	425016	564940
Norwich Centre	URBAN CENTRE	623000	308900
Nottingham Centre	URBAN CENTRE	457452	340103
Plymouth Centre	URBAN CENTRE	247742	54600
Rotherham Centre	URBAN CENTRE	443000	393000
Sheffield Centre	URBAN CENTRE	435134	386885
Southampton Centre	URBAN CENTRE	442575	112260
Stoke-on-Trent Centre	URBAN CENTRE	388348	347894
Swansea	URBAN CENTRE	265566	193158
Wolverhampton Centre	URBAN CENTRE	391368	298942

Site	Site type	East	North
Grangemouth	URBAN INDUSTRIAL	293840	681032
Middlesbrough	URBAN INDUSTRIAL	450480	519632
Ribble Valley Chatburn	URBAN INDUSTRIAL	377950	444350
Salford Eccles	URBAN INDUSTRIAL	377932	398743
Scunthorpe	URBAN INDUSTRIAL	490592	410689

Appendix 4: Spatial analysis of meteorological data

Introduction

Dispersion models used for the assessment of the impacts of large industrial sources on ambient air concentrations of pollutants usually make use of hourly sequential meteorological data from sites throughout the UK. The number of sites available is limited, so the emission source and receptor locations may be some distance from the nearest meteorological station. This investigation was carried out to assess the effect of the distance of the meteorological station on predicted concentrations.

Meteorological data

Hourly sequential meteorological data for 1999, suitable for use in dispersion models was obtained from the Meteorological Office for eleven sites throughout England and Wales.

Table A4.1: Coordinates of meteorological stations

Site	OS grid coordinates, 100 m units	
	Easting	Northing
Boulmer	4265	6145
Coleshill	4195	2895
Heathrow	5075	1755
Hurn	4125	965
London Weather Centre	5301	1805
Ringway	3815	3845
Shawbury	3545	3225
Valley	2305	3755
Waddington	4985	3645
Wattisham	6025	2515
Yeovilton	3543	1231

The data provided details of cloud cover, wind direction and wind speed for each hour of the year at each site.

Variograms

Variograms were calculated for cloud cover, wind direction and wind speed as follows. For each pair of meteorological stations, the variance of each pair of hourly data values, (x_1, x_2) was calculated:

$$s^2 = \frac{(x_1 - x_2)^2}{2}$$

For the wind direction data, the difference x_1-x_2 was replaced with min{x_1-x_2, 180-(x_1-x_2)}.

A pooled estimate of the variance over all hours was then obtained for each pair of sites as the mean of the variance estimates. The standard deviation was calculated as the square root of the pooled variance estimate. The standard deviation calculated for each pair of sites was then plotted against the distance between the sites.

FigureA4.1 shows the variogram for hourly cloud cover. The variogram shows that the difference between cloud cover estimates at pairs of sites increases with increasing distance between sites (as might be expected). The standard deviation appears to approach a residual or 'nugget' value of approximately 0.75 oktas as the distance between sites approaches zero. This nugget contains components associated with the error in the cloud cover estimate and possible local-scale microvariability.

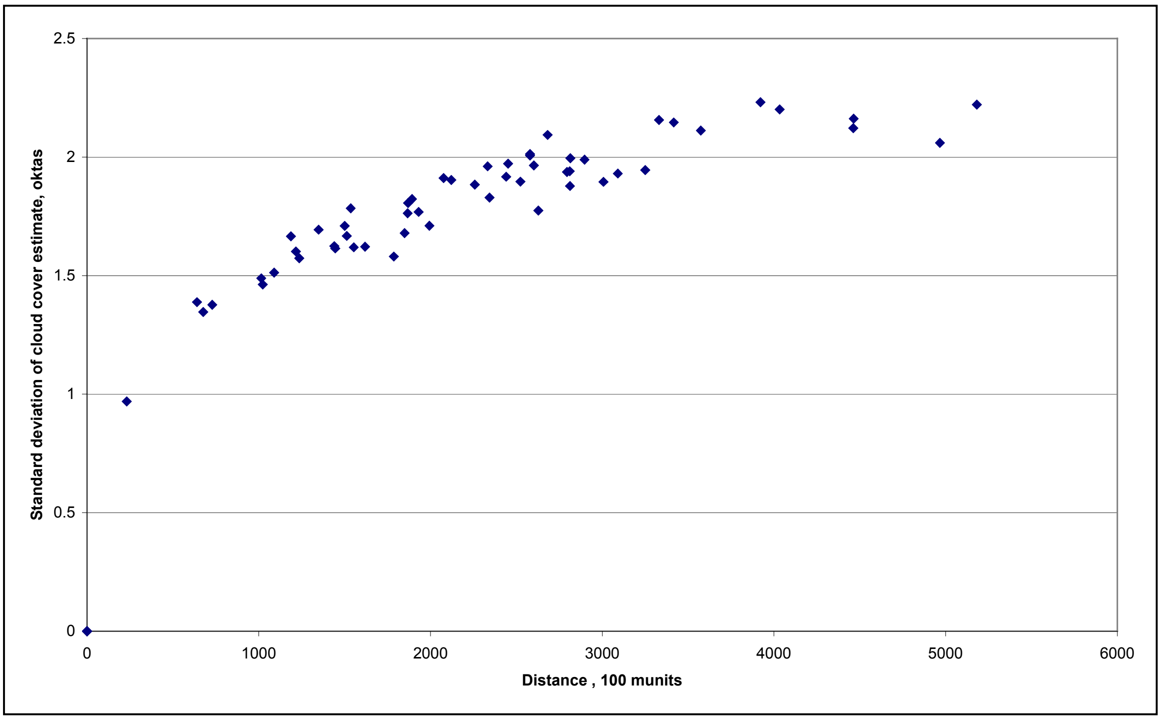


Figure A4.1: Cloud cover variogram

Figure A4.2 shows the variogram for hourly wind direction. The variogram shows that the difference between wind direction measurements at pairs of sites increases with increasing distance between sites (as might be expected). The standard deviation appears to approach a residual or 'nugget' value of approximately 20 degrees as the distance between sites approaches zero.

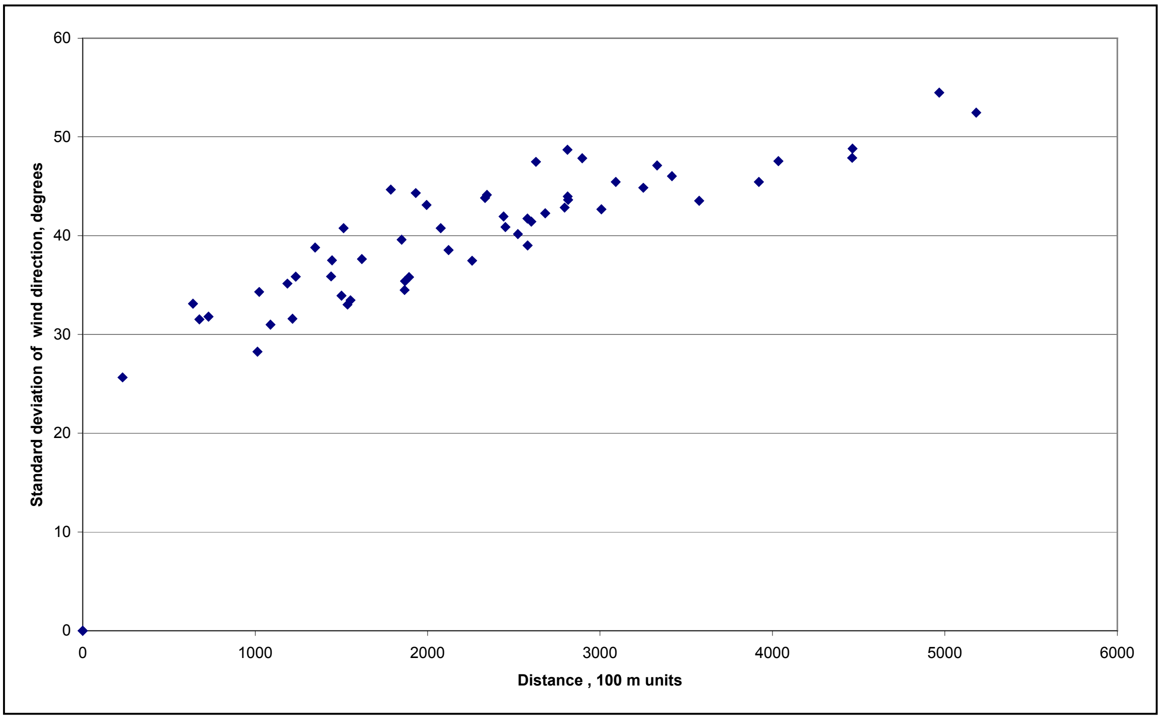


Figure A4.2: Wind direction variogram

Figure A4.3 shows the variogram for hourly wind speed. The variogram shows a general trend of the standard deviation of wind speed pairs increasing with distance between the meteorological data sites. There are a number of outlying points above the general trend: in each case the outlying point is associated with the Valley meteorological station. The Valley station is located at an exposed coastal location with high wind speeds that are not typical of the other, generally more inland, sites. Excluding the Valley data, the variogram shows that the difference between wind speed measurements at pairs of sites increases with increasing distance between sites (as might be expected). The standard deviation appears to approach a residual or 'nugget' value of approximately 0.75 m s^{-1} as the distance between sites approaches zero.

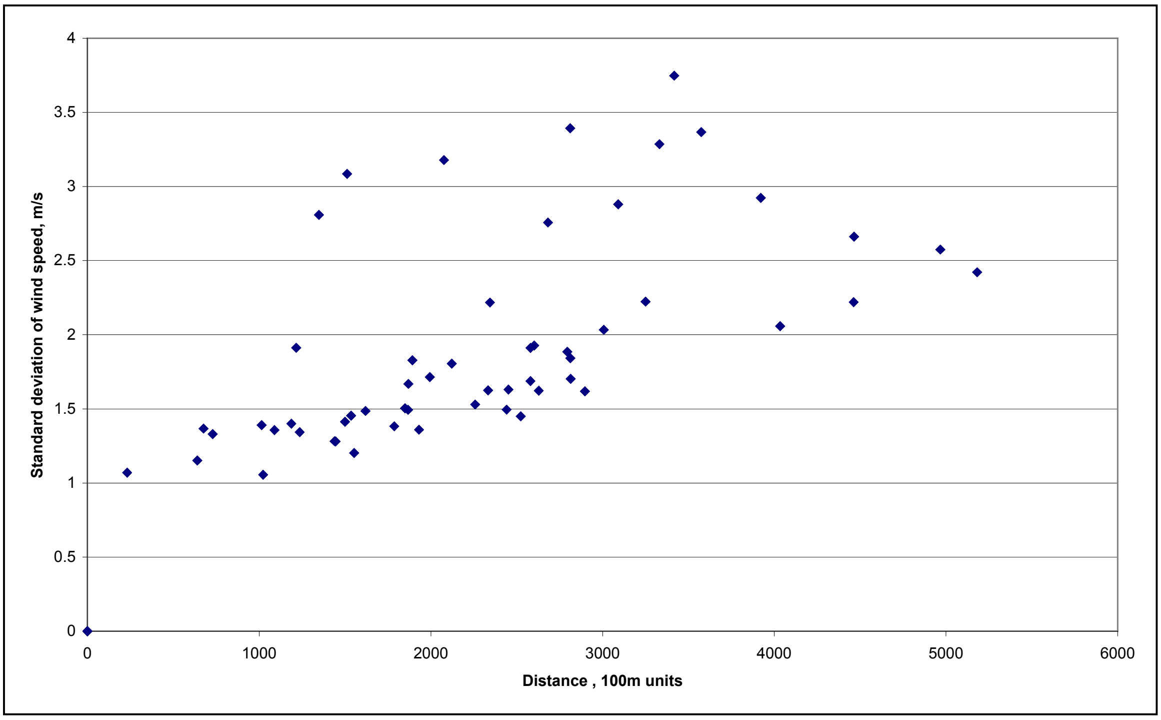


Figure A4.3: Wind speed variogram

Dispersion modelling

The dispersion model ADMS 3.1 was used to determine maximum ground level concentrations from a typical industrial stack emission using each of the meteorological data sets in turn. Table A4.2 shows the model input parameters. Table A4.3 shows the predicted maximum annual average concentrations and the 99.9th percentile of 15-minute mean concentrations predicted using each of the meteorological data sets. The predicted concentrations do not appear to have any spatial pattern and are similar in each case. The meterological data set for Valley results in the highest predicted annual average concentration, possibly as a result of the higher wind speeds at this location.

Table A4.2: Model input parameters

Input parameter	**Value**
Stack height	100 m
Stack diameter	2 m
Discharge temperature	130 °C
Discharge velocity	15 m s^{-1} actual
Surface roughness	0.1 m
Emission	1 g s^{-1}
Receptor grid dimension	6 km x 6 km centred on the stack
Receptor spacing	100 m

Table A4.3: Modelled maximum ground level concentrations

Meteorological data	99.9th percentile of 15-minute mean concentrations, μg m^{-3}	Annual mean, μg m^{-3}
Boulmer	1.86	0.039
Coleshill	1.97	0.038
Heathrow	2.26	0.036
Hurn	1.72	0.039
London Weather Centre	1.72	0.040
Ringway	2.35	0.038
Shawbury	1.94	0.046
Valley	1.99	0.061
Waddington	1.90	0.045
Wattisham	1.80	0.034
Yeovilton	2.00	0.042

Conclusions

1) The error in the estimated cloud cover, wind direction and wind speed increases as the distance of the meteorological station from the receptor area/source location increases.
2) The error in the estimated cloud cover, wind direction and wind speed decreases to a finite residual or nugget value (greater than zero) as the distance from the meteorological station approaches zero. The residual error may be associated with measurement errors or local microscale variation.
3) The wind speed in particular may be influenced by local topographical features (the coastline, for example), so that proximity to the receptor area should not be the sole criterion when selecting meteorological data for dispersion modelling.
4) The choice of meteorological data site has a relatively small effect on the predicted maximum ground level concentrations. The coefficients of variation of the maximum predicted annual means and 99.9 th percentile 15-minute means were 18 per cent and 10 per cent respectively.

Appendix 5: Emission characteristics of large oxides of nitrogen sources

PlantID	Authorisation	Site	Emission(g/s)	Height_m	Diameter_m	Vel_m/s	Temp_C	OS_GRE	OS_GRN
44	AA2534	Ferrybridge C	497.12	198	10.00	19.40	130	446700	424800
45	AA3301	Fiddlers Ferry	326.39	199	13.00	19.00	125	354300	386500
51	AA2488	Drax	1571.73	259	15.83	30.02	90	466400	426400
52	BA9436	Fifoots Point	16.90	145.20	8.30	18.39	128	332800	183800
120	AA2011	Ashington	244.95	114.30	6.07	15.24	140	430600	590200
150	AF8408	Roosecote	27.28	40	3.00	15.00	150	322300	468400
322	AA2348	Seal Sands	62.74	76	2.30	18.00	220	453400	524000
367	AI0608	Hope	142.91	132	4.50	12.95	138	416900	382200
369	AH9529	Cauldon	56.37	106	3.13	19.20	100	408500	349600
370	AI0497	Weardale	22.43	122	2.79	22.30	112	394500	537500
372	AI0322	Westbury	96.97	122	3.70	10.23	165	388620	152640
373	AH9499	Northfleet	191.24	122	2.79	22.30	112	563600	174400
374	AI0713	Aberthaw	26.04	46	3.00	15.00	150	303400	167500
425	AA3387	Coryton A	11.78	106.70	2.43	19.10	160	574400	182300
425	AA3387	Coryton B	16.41	106.70	2.43	19.10	160	574400	182300
425	AA3387	Coryton C	7.05	45.70	2.43	7.69	182	574400	182300
425	AA3387	Coryton D	7.05	45.70	2.43	7.69	182	574400	182300
425	AA3387	Coryton E	21.04	91.40	4.10	9.30	254	574400	182300
425	AA3387	Coryton F	3.28	51.80	1.60	7.31	277	574400	182300
425	AA3387	Coryton G	14.58	117	2.90	11.64	203	574400	182300
425	AA3387	Coryton H	13.13	80.20	4.05	4.87	160	574400	182300
458	AA2470	Eggborough	449.69	198	12.00	27.00	130	457500	424500
467	AM1461	Kings Lynn	18.13	40	3.00	15.00	150	561300	317600
469	AF9706	Peterborough	34.25	60	4.80	26.97	150	521800	299200
534	AH9847	Tunstead	50.38	40	3.00	15.00	150	410000	374500

PlantID	Authorisation	Site	Emission(g/s)	Height_m	Diameter_m	Vel_m/s	Temp_C	OS_GRE	OS_GRN
564	AI2813	Clitheroe	64.67	104.50	4.20	12.67	220	375200	443700
565	AI0349	Padeswood	33.87	41	2.40	15.00	150	329100	362400
709	AF8173	South Killingholme	21.91	92	4.23	9.04	520	516100	416500
709	AF8173	South Killingholme	15.52	64	1.67	17.00	475	516100	416500
709	AF8173	South Killingholme	7.83	115	2.80	18.78	272	516100	416500
709	AF8173	South Killingholme	14.61	92	2.44	21.70	605	516100	416500
709	AF8173	South Killingholme	70.70	122	5.94	18.70	570	516100	416500
739	AG6621	Corby	64.49	70	6.25	16.01	150	489600	291100
741	AA2216	Scunthorpe	20.99	96	3.80	14.81	200	492000	409500
741	AA2216	Scunthorpe	17.67	76.50	4.24	17.19	176	492000	409500
742	AF7193	Scunthorpe	1.75	76	3.75	5.00	300	492000	409500
742	AF7193	Scunthorpe	28.15	76	3.75	5.00	300	492000	409500
744	AR0080	Scunthorpe	11.19	107	6.40	15.45	160	492000	409500
744	AR0080	Scunthorpe	125.15	107	6.40	15.45	160	492000	409500
744	AR0080	Scunthorpe	1.37	107	6.40	15.45	160	492000	409500
751	AA2950	Redcar	37.93	115.50	3.02	20.50	200	456730	525690
755	AF8548	Redcar	1.48	60	1.98	10.60	293	456290	525880
755	AF8548	Redcar	23.79	60	1.98	10.60	293	456290	525880
757	AF8866	Redcar	9.05	70	2.50	10.50	270	457700	524200
757	AF8866	Redcar	13.81	61.50	2.23	14.70	760	457700	524200
757	AF8866	Redcar	10.79	57	3.00	17.40	500	457700	524200
757	AF8866	Redcar	10.10	33	1.23	5.00	300	457700	524200
759	AR0241	Teesside	1.21	115.50	3.00	20.50	200	456730	525690
759	AR0241	Teesside	93.75	115.50	3.00	20.50	200	456730	525690
759	AR0241	Teesside	9.57	115.50	3.00	20.50	200	456730	525690
760	AF8238	Rotherham	35.23	65	3.00	15.00	150	444800	395100
770	AA2631	Llanwern	15.94	82.30	2.97	18.50	164	336900	186700
770	AA2631	Llanwern	21.92	51.80	2.59	25.70	183	336900	186700
777	AA2780	Port Talbot	18.75	121	3.89	10.77	200	278200	187000
777	AA2780	Port Talbot	18.75	37	2.70	7.16	210	278200	187000
778	AF8645	Morfa	69.62	127	4.70	4.50	230	277900	187100
778	AF8645	Morfa	4.33	127	4.70	4.50	230	277900	187100
781	AR0357	Port Talbot	5.93	74	4.95	9.57	190	278200	187000

PlantID	Authorisation	Site	Emission(g/s)	Height_m	Diameter_m	Vel_m/s	Temp_C	OS_GRE	OS_GRN
781	AR0357	Port Talbot	0.82	31	2.94	10.40	145	278200	187000
781	AR0357	Port Talbot	53.43	133	8.35	7.25	123	278200	187000
783	AZ6967	Cottam Development Centre	20.53	198	15.80	17.40	130	481700	379700
784	AA3433	Cottam	554.54	198	15.80	18.00	125	481700	379700
847	AJ2992	London	22.40	38	2.00	10.00	125	539250	179050
849	BB8982	Damhead Creek	47.53	75	8.00	15.00	150	581000	172800
852	AI5944	Deeside	29.03	53	3.00	15.00	150	329700	371400
879	AE1203	Derwent	30.01	60	4.00	15.00	100	439500	335100
964	AF7886	Milford Haven	27.50	110	4.00	18.30	276	188600	208700
964	AF7886	Milford Haven	1.72	100	1.60	8.31	250	188600	208700
964	AF7886	Milford Haven	28.08	110	4.24	8.83	230	188600	208700
984	AA8397	Greystones	135.88	45	3.00	14.00	109	456530	520390
986	AA3069	Wilton	35.78	91	3.05	14.30	135	456910	521970
986	AA3069	Wilton	35.78	137	4.88	16.04	135	456910	521970
986	AA3069	Wilton	54.11	187	3.00	11.60	350	456910	521970
986	AA3069	Wilton	52.33	104	3.00	11.60	300	456910	521970
996	AF8009	Fawley	34.86	107	3.00	15.00	200	444300	103800
996	AF8009	Fawley	35.82	73	3.00	15.00	200	444300	103800
996	AF8009	Fawley	40.06	137	3.00	15.00	200	444300	103800
996	AF8009	Fawley	20.80	37	3.00	15.00	200	444300	103800
996	AF8009	Fawley	39.48	62	3.00	15.00	200	444300	103800
996	AF8009	Fawley	21.57	63	3.00	15.00	200	444300	103800
1285	AH4195	South Humber	95.43	75	7.00	15.00	150	522500	413300
1291	AK7868	Redcar	8.21	104	3.00	11.60	300	458000	521100
1291	AK7868	Redcar	5.61	91	3.05	14.30	135	458000	521100
1291	AK7868	Redcar	5.61	137	4.88	16.04	135	458000	521100
1291	AK7868	Redcar	8.49	187	3.00	11.60	350	458000	521100
1364	AA3123	Runcorn	24.24	40	3.00	15.00	150	350200	380300
1390	AJ2747	Little Barford	50.07	65	8.00	15.00	150	518500	257700
1394	AA3204	Tilbury B	592.57	171	6.30	19.06	140	566200	175600
1403	AA3166	Littlebrook D	17.75	215	11.30	31.00	140	555800	176500
1404	AA3107	Didcot A	494.33	198	12.00	20.55	150	451300	191900
1405	AO4003	Didcot B	56.85	85	9.20	20.00	94	450400	192300

PlantID	Authorisation	Site	Emission(g/s)	Height_m	Diameter_m	Vel_m/s	Temp_C	OS_GRE	OS_GRN
1407	AA2682	Aberthaw B	720.97	152	6.80	23.40	126	302300	166000
1493	AB4745	Keadby	22.25	60	3.00	15.00	150	483500	411500
1499	AF0920	Killingholme	62.46	65	5.50	15.00	100	513500	417500
1525	AI0438	Whitwell	86.16	96	4.00	15.00	150	454000	374700
1573	AF6928	Killingholme	19.55	98	4.10	10.50	230	515800	417700
1573	AF6928	Killingholme	9.73	91	2.70	17.50	350	515800	417700
1573	AF6928	Killingholme	39.19	137	4.70	12.50	245	515800	417700
1573	AF6928	Killingholme	18.42	132	3.99	10.56	205	515800	417700
1580	AG5269	Edmonton	27.69	100	2.70	13.20	140	535800	192600
1633	AA6823	Medway	16.24	60	3.00	15.00	150	588700	175600
1671	AF7835	Barnsley	1.33	45	1.83	15.00	150	437600	412200
1671	AF7835	Barnsley	21.30	45	1.83	15.00	150	437600	412200
1810	AF7215	North Tees	19.35	40	3.00	15.00	150	452960	523080
1822	AF6847	Norwich	52.98	30	2.00	15.00	150	632800	334800
1865	AB5873	Killingholme	35.52	76	6.80	20.00	107	514000	418800
1868	AA2267	Ratcliffe on Soar	723.76	199	11.90	23.50	80	450400	329700
1870	AA3000	Kingsnorth	522.85	198	12.20	26.00	130	580600	172200
1875	AP5790	Connahs Quay	29.66	85	7.40	15.00	92	327900	371000
1924	AA6904	Brigg	23.96	65	3.00	15.00	150	498700	406200
2027	AT6476	Rocksavage	30.71	75	8.00	15.00	150	349700	381500
2069	AP8314	New Rugby	44.36	115	8.00	15.00	150	448900	275800
2071	AH8727	Rochester	31.69	114	7.07	4.28	150	570300	165100
2076	AA2658	Rugeley B	209.78	183	8.80	23.00	130	405900	317100
2090	BA2814	Saltend	100.64	65	6.00	25.00	90	516100	427800
2121	AG8411	Rye House	44.59	65	6.70	15.50	150	538800	280000
2125	AR1051	Seabank	51.48	65	8.00	15.00	150	355000	180300
2145	AF7916	Avonmouth	21.04	46	2.01	26.50	223	353470	181630
2165	AF8394	Stanlow	5.20	75	2.60	4.80	225	343800	375800
2165	AF8394	Stanlow	14.31	125	1.00	4.40	280	343800	375800
2165	AF8394	Stanlow	6.50	122	5.00	4.60	230	343800	375800
2165	AF8394	Stanlow	54.62	155	7.45	10.10	175	343800	375800
2165	AF8394	Stanlow	42.92	80	3.50	13.10	160	343800	375800
2165	AF8394	Stanlow	6.50	143	4.00	4.40	175	343800	375800

PlantID	Authorisation	Site	Emission(g/s)	Height_m	Diameter_m	Vel_m/s	Temp_C	OS_GRE	OS_GRN
2180	BA1931	Shoreham	20.47	46	3.00	15.00	150	524600	104800
2230	AE7236	SELCHP	18.08	100	2.10	20.00	120	535700	178120
2326	AL7561	Billingham	5.61	41	2.90	18.10	150	447070	522410
2326	AL7561	Billingham	44.36	41	2.90	18.10	150	447070	522410
2327	AN8321	Billingham	43.44	41	2.90	18.10	150	447210	522410
2339	AF7894	Pembroke	10.63	162	2.97	8.79	160	191000	202300
2339	AF7894	Pembroke	16.24	167	4.38	6.16	230	191000	202300
2339	AF7894	Pembroke	11.66	92	3.30	7.83	180	191000	202300
2339	AF7894	Pembroke	14.51	92	2.70	14.50	180	191000	202300
2339	AF7894	Pembroke	33.34	158	3.95	15.61	156	191000	202300
2345	AB3838	Barking	26.28	55	8.70	23.70	127	549000	182300
2417	AK2815	Knapton	33.94	46	3.00	15.00	150	488700	477000
2421	AA3212	West Burton	514.46	183	8.90	25.00	125	479100	385700
2422	AA2674	Ironbridge	358.08	204	8.58	27.60	130	365400	303800
2423	AA2925	Drakelow C	164.46	168	8.10	10.40	144	424000	319500
2424	AA3425	High Marnham	180.78	137	11.70	16.00	132	485700	370600
2425	AS9216	Tyseley	16.89	80	2.10	18.50	140	410900	284500
2590	0087/99A	Cookstown	30.92	40	3.00	15.00	150	89567	539888
2591	IPC/E/00016	Dunbar	35.17	40	3.00	15.00	150	370240	675640
2601	IPC/E/00039	Cockenzie	337.92	149	7.35	22.00	132	340000	675000
2602	IPC/E/00069	Longannet	749.58	183	15.12	18.60	110	300000	687000
2605	0011/98A	Kilroot	104.53	198	12.00	20.00	150	154500	541000
2605	0011/98A	Kilroot	116.94	200	5.50	17.64	120	154500	541000
2606	0007/98A	Coolkeeragh	4.45	81	3.80	15.00	150	62000	584500
2606	0007/98A	Coolkeeragh	6.03	81	4.42	15.00	150	62000	584500
2606	0007/98A	Coolkeeragh	4.45	81	3.80	15.00	150	62000	584500
2606	0007/98A	Coolkeeragh	7.73	198	12.00	20.00	150	62000	584500
2607	0008/98A	Ballylumford	4.11	124	5.90	15.00	140	157900	558000
2607	0008/98A	Ballylumford	4.11	124	5.90	15.00	140	157900	558000
2607	0008/98A	Ballylumford	4.11	124	5.90	15.00	140	157900	558000
2607	0008/98A	Ballylumford	95.74	198	12.00	20.00	150	157900	558000
2608	IPC/N/20019	Peterhead	63.06	165	9.40	20.00	145	412000	845000
3081	IPC/E/00011	Grangemouth	173.28	100	3.00	15.00	150	294351	680627

PlantID	Authorisation	Site	Emission(g/s)	Height_m	Diameter_m	Vel_m/s	Temp_C	OS_GRE	OS_GRN
3960		Arpley Landfill Site	35.33	46	3.00	15.00	150	358231	386365
3984		Brogborough Power Station (Phase I & II)	23.97	40	3.00	15.00	150	496887	240383
4044		LField Stewartby	26.56	40	3.00	15.00	150	501391	243408
4074		Packington Gas Control Plant	17.77	40	3.00	15.00	150	420831	285122
4090		Rainham Phase II	23.40	40	3.00	15.00	150	552737	179296
4171		Davyhulme CHP at Davyhulme WWTW	18.96	40	3.00	15.00	150	375400	396400
4186		Minworth Generating Station	25.08	40	3.00	15.00	150	416086	292301
4187		Mogden Sewage Treatment Works	27.75	40	3.00	15.00	150	514844	174804
4339	BJ7891	Baglan Bay	29.43	162	3.70	11.81	190	273100	192400
4359	BK0973	Barrington	34.86	53	3.00	15.00	150	539580	250280
4402	BL1029	South Ferriby	57.04	53	3.00	15.00	150	497300	420900
4426	BM0486	Ketton	80.17	53	3.00	15.00	150	498470	305320
5142		Shelford Generation Plant II	17.34	46	3.00	15.00	150	615958	160346

Appendix 6: Monitoring sites used to calibrate and verify the mapped estimates

Table A6.1: National network monitoring sites operating during 2002

Station code	Local station code	Zone code	Zone	Use for Directive				Use for Directive / Measuring method
				SO_2	NO_2	NO_x	Lead	PM_{10}
GB0729A	Aberdeen	UK0038	North East Scotland	+	+			M3
	Avesta Polarit Rotherham	UK0007	Sheffield Urban Area				+	
GB0600A	Barnsley 12	UK0034	Yorkshire & Humberside	+				
GB0681A	Barnsley Gawber	UK0034	Yorkshire & Humberside	+	+			
GB0647A	Bath Roadside	UK0030	South West		+			
GB0567A	Belfast Centre	UK0028	Belfast Urban Area	+	+			M3
GB0696A	Belfast Clara St	UK0028	Belfast Urban Area					M1
GB0514A	Belfast East	UK0028	Belfast Urban Area	+				
GB0421A	Billingham	UK0013	Teesside Urban Area		+			
GB0569A	Birmingham Centre	UK0002	West Midlands Urban Area	+	+			M3
GB0595A	Birmingham East	UK0002	West Midlands Urban Area	+	+			M3
GB0727A	Blackpool	UK0022	Blackpool Urban Area	+	+			M3
GB0654A	Bolton	UK0003	Greater Manchester Urban Area	+	+			M3
GB0741A	Bournemouth	UK0015	Bournemouth Urban Area	+	+			M2
GB0689A	Bradford Centre	UK0004	West Yorkshire Urban Area	+	+			M3
GB0693A	Brighton Roadside	UK0010	Brighton/Worthing/Littlehampton		+			
GB0585A	Bristol Centre	UK0009	Bristol Urban Area	+	+			M3
GB0639A	Bristol Old Market	UK0009	Bristol Urban Area		+			
	Britannia Recycling Wakefield	UK0004	West Yorkshire Urban Area				+	
GB0417A	Brookside 2 lead site	UK0002	West Midlands Urban Area				+	
GB0652A	Bury Roadside	UK0003	Greater Manchester Urban Area	+	+			M3
GB0789A	BZL Hallen	UK0030	South West				+	
GB0726A	Cambridge Roadside	UK0029	Eastern		+			
GB0636A	Camden Kerbside	UK0001	Greater London Urban Area		+			M3
GB0737A	Canterbury	UK0031	South East		+			M3
GB0580A	Cardiff Centre	UK0026	Cardiff Urban Area	+	+			M3
GB0369A	Cardiff lead site	UK0026	Cardiff Urban Area				+	

Station code	Local station code	Zone code	Zone	Use for Directive				Use for Directive / Measuring method
				SO_2	NO_2	NO_x	Lead	PM_{10}
GB0537A	Central London lead site	UK0001	Greater London Urban Area				+	
GB0194A	Chilton lead site	UK0031	South East				+	
GB0739A	Coventry Memorial Park	UK0017	Coventry/Bedworth	+	+			M3
GB0744A	Cwmbran	UK0041	South Wales	+	+			M3
GB0673A	Derry	UK0043	Northern Ireland	+	+			M3
GB0740A	Dumfries	UK0040	Scottish Borders		+			M2
GB0581A	Edinburgh Centre	UK0025	Edinburgh Urban Area	+	+			M3
GB0419A	Elswick 6 lead site	UK0005	Tyneside				+	
GB0361A	Eskdalemuir lead site	UK0040	Scottish Borders				+	
GB0640A	Exeter Roadside	UK0030	South West	+	+			
GB0641A	Glasgow Centre	UK0024	Glasgow Urban Area	+	+			M3
GB0452A	Glasgow City Chambers	UK0024	Glasgow Urban Area		+			
GB0657A	Glasgow Kerbside	UK0024	Glasgow Urban Area		+			M3
GB0260A	Glasgow lead site	UK0024	Glasgow Urban Area				+	
GB0735A	Grangemouth	UK0037	Central Scotland	+	+			M3
GB0637A	Haringey Roadside	UK0001	Greater London Urban Area		+			M3
GB0036R	Harwell	UK0031	South East	+	+	+		
GB0685A	Hounslow Roadside	UK0001	Greater London Urban Area		+			
GB0686A	Hove Roadside	UK0010	Brighton/Worthing/Littlehampton	+	+			
GB0776A	Hull Freetown	UK0018	Kingston upon Hull	+	+			M3
GB0382A	IMI 2 lead site	UK0002	West Midlands Urban Area				+	
GB0742A	Inverness	UK0039	Highland		+			M2
GB0037R	Ladybower	UK0032	East Midlands	+	+			
GB0643A	Leamington Spa	UK0035	West Midlands	+	+			M3
GB0584A	Leeds Centre	UK0004	West Yorkshire Urban Area	+	+			M3
GB0248A	Leeds lead site	UK0004	West Yorkshire Urban Area				+	
GB0597A	Leicester Centre	UK0011	Leicester Urban Area	+	+			M3
GB0659A	London A3 Roadside	UK0001	Greater London Urban Area		+			M3
GB0608A	London Bexley	UK0001	Greater London Urban Area	+	+			M3
GB0566A	London Bloomsbury	UK0001	Greater London Urban Area	+	+			M3

Station code	Local station code	Zone code	Zone	Use for Directive				Use for Directive / Measuring method
				SO_2	NO_2	NO_x	Lead	PM_{10}
GB0616A	London Brent	UK0001	Greater London Urban Area	+	+			M3
GB0635A	London Brent Park lead site	UK0001	Greater London Urban Area				+	
GB0697A	London Bromley	UK0001	Greater London Urban Area		+			
GB0695A	London Cromwell Road 2	UK0001	Greater London Urban Area	+	+			
GB0332A	London Cromwell Road lead site	UK0001	Greater London Urban Area				+	
GB0586A	London Eltham	UK0001	Greater London Urban Area	+	+			M3
GB0650A	London Hackney	UK0001	Greater London Urban Area		+			
GB0642A	London Hillingdon	UK0001	Greater London Urban Area	+	+			M3
GB0672A	London Lewisham	UK0001	Greater London Urban Area	+	+			
GB0682A	London Marylebone Road	UK0001	Greater London Urban Area	+	+			M3
GB0620A	London N. Kensington	UK0001	Greater London Urban Area	+	+			M3
GB0656A	London Southwark	UK0001	Greater London Urban Area	+	+			
GB0644A	London Teddington	UK0001	Greater London Urban Area	+	+			
GB0622A	London Wandsworth	UK0001	Greater London Urban Area		+			
GB0743A	London Westminster	UK0001	Greater London Urban Area	+	+			
GB0006R	Lough Navar	UK0043	Northern Ireland					M3
GB0038R	Lullington Heath	UK0031	South East	+	+			
GB0370A	Manchester lead site	UK0003	Greater Manchester Urban Area				+	
GB0613A	Manchester Piccadilly	UK0003	Greater Manchester Urban Area	+	+			M3
GB0649A	Manchester South	UK0003	Greater Manchester Urban Area	+	+			
GB0453A	Manchester Town Hall	UK0003	Greater Manchester Urban Area		+			
GB0583A	Middlesbrough	UK0013	Teesside Urban Area	+	+			M3
GB0241A	Motherwell lead site	UK0024	Glasgow Urban Area				+	
GB0043R	Narberth	UK0041	South Wales	+	+	+		M3
GB0568A	Newcastle Centre	UK0005	Tyneside	+	+			M3
GB0738A	Northampton	UK0032	East Midlands	+	+			M3,M2
GB0684A	Norwich Centre	UK0029	Eastern	+	+			M3
GB0678A	Norwich Roadside	UK0029	Eastern		+			
GB0646A	Nottingham Centre	UK0008	Nottingham Urban Area	+	+			M3

Station code	Local station code	Zone code	Zone	Use for Directive				Use for Directive / Measuring method
				SO_2	NO_2	NO_x	Lead	PM_{10}
GB0633A	Oxford Centre	UK0031	South East	+	+			
GB0687A	Plymouth Centre	UK0030	South West	+	+			M3
GB0198A	Pontardawe lead site	UK0041	South Wales				+	
GB0651A	Port Talbot	UK0027	Swansea Urban Area	+	+			M3
GB0733A	Portsmouth	UK0012	Portsmouth Urban Area	+	+			M3
GB0731A	Preston	UK0023	Preston Urban Area	+	+			M3
GB0683A	Reading	UK0016	Reading/Wokingham Urban Area	+	+			M3
GB0679A	Redcar	UK0013	Teesside Urban Area	+	+			M3
GB0617A	Rochester	UK0031	South East	+	+			M3
GB0677A	Rotherham Centre	UK0007	Sheffield Urban Area	+	+			
GB0660A	Salford Eccles	UK0003	Greater Manchester Urban Area	+	+			M3
GB0698A	Sandwell West Bromwich	UK0002	West Midlands Urban Area	+	+			
GB0690A	Scunthorpe	UK0034	Yorkshire & Humberside	+				M3
GB0615A	Sheffield Centre	UK0007	Sheffield Urban Area	+	+			M3
GB0538R	Sheffield Tinsley	UK0007	Sheffield Urban Area		+			
GB0598A	Southampton Centre	UK0019	Southampton Urban Area	+	+			M3
GB0728A	Southend-on-Sea	UK0021	Southend Urban Area	+	+			M3
GB0667A	Southwark Roadside	UK0001	Greater London Urban Area	+	+			
GB0754A	St Osyth	UK0029	Eastern		+	+		
GB0775A	Stockport Shaw Heath	UK0003	Greater Manchester Urban Area	+	+			M3
GB0734A	Stockton-on-Tees Yarm	UK0036	North East		+			M3
GB0658A	Stoke-on-Trent Centre	UK0014	The Potteries	+	+			M3
GB0193A	Styrrup lead site	UK0032	East Midlands				+	
GB0582A	Sunderland	UK0036	North East	+				
GB0609A	Swansea	UK0027	Swansea Urban Area	+	+			M3
GB0645A	Thurrock	UK0029	Eastern	+	+			M3
GB0642A	Tower Hamlets Roadside	UK0001	Greater London Urban Area		+			
GB0455A	Walsall Alumwell	UK0002	West Midlands Urban Area		+			
GB0674A	Walsall Willenhall	UK0002	West Midlands Urban Area		+			
GB0420A	West London	UK0001	Greater London Urban Area		+			

Station code	Local station code	Zone code	Zone	Use for Directive				Use for Directive / Measuring method
				SO_2	NO_2	NO_x	Lead	PM_{10}
GB0045R	Wicken Fen	UK0029	Eastern	+	+	+		
GB0736A	Wigan Leigh	UK0033	North West & Merseyside	+	+			M3
GB0730A	Wirral Tranmere	UK0020	Birkenhead Urban Area	+	+			M3
GB0614A	Wolverhampton Centre	UK0002	West Midlands Urban Area	+	+			M3
GB0192A	Wraymires lead site	UK0033	North West & Merseyside				+	
GB0755A	Wrexham	UK0042	North Wales	+	+			M2

+ = monitoring for the Directive at that site

M1 = Beta attenuation monitor, M2 =Gravimetric, M3 = TEOM measurements for PM_{10}

Table A6.2: Additional monitoring sites used to verify the mapped estimates (all PM_{10} measurements by TEOM).

Site	Authority or Company	Site Type	SO_2	NO_2	PM_{10}
Abingdon	Vale of White Horse DC	URBAN BACKGROUND	+	+	+
Bacton Gas Terminal	BP Amoco Exploration	RURAL		+	
Birmingham Airport	Birmingham International Airport	URBAN BACKGROUND	+	+	+
Bracknell Bagshot Road	Bracknell Forest BC	ROADSIDE		+	+
Bracknell Foxhill	Bracknell Forest BC	URBAN BACKGROUND		+	
Brentwood	Brentwood BC	URBAN BACKGROUND		+	
Cambridge Gonville Place	Cambridge City Council	ROADSIDE		+	+
Gatwick LGW3	BAA	URBAN BACKGROUND		+	+
Heathrow Bedfont Court	BAA	URBAN BACKGROUND			+
Heathrow Green Gates	BAA	URBAN BACKGROUND		+	+
Heathrow LHR2	BAA	URBAN BACKGROUND		+	+
Heathrow Main Road	BAA	URBAN BACKGROUND	+	+	+
Heathrow Moorbridge	BAA	URBAN BACKGROUND			+
Heathrow Oaks Road	BAA	URBAN BACKGROUND			+
Liverpool Islington	Liverpool City Council	ROADSIDE	+	+	+
Liverpool Vauxhall	Liverpool City Council	URBAN BACKGROUND	+	+	+
Liverpool Victoria Street	Liverpool City Council	ROADSIDE	+	+	+
Newham Cam Road	London Borough of Newham	ROADSIDE	+	+	+

Site	Authority or Company	Site Type	SO_2	NO_2	PM_{10}
Newham Tant Avenue	London Borough of Newham	URBAN BACKGROUND	+	+	+
Newry Monaghan Row	Newry and Mourne DC	URBAN BACKGROUND	+		+
Newry Trevor Hill	Newry and Mourne DC	ROADSIDE	+		
Oldham West Endhouse	Oldham Metropolitan Borough Council	URBAN BACKGROUND	+	+	+
Oxford East	Oxford City Council	URBAN BACKGROUND		+	+
Oxford St Ebbes	Oxford City Council	URBAN BACKGROUND		+	+
Ribble Valley Chatburn	Ribble Valley Borough Council	RURAL	+	+	+
Ribble Valley Lillands	Ribble Valley Borough Council	RURAL	+	+	+
Salford M60	Salford MBC	ROADSIDE	+	+	+
Slough Colnbrook	Slough Borough Council	URBAN BACKGROUND		+	+
Slough Town Centre A4	Slough Borough Council	ROADSIDE		+	+
South Bucks Gerrards Cross	South Bucks District Council	KERBSIDE		+	+
South Cambs Bar Hill	South Cambridgeshire DC	KERBSIDE		+	
South Holland	South Holland DC	URBAN BACKGROUND		+	+
Stockport Bredbury	Stockport Metropolitan BC	URBAN BACKGROUND		+	+
Stockport Cheadle	Stockport Metropolitan BC	URBAN BACKGROUND		+	+
Stockport Marple	Stockport Metropolitan BC	URBAN BACKGROUND		+	+
Strabane Springhill Park	Strabane DC	URBAN BACKGROUND	+		
Sutton Bridge (Petts Lane)	South Holland DC	URBAN BACKGROUND			+
Tameside Two Trees School	Tameside Metropolitan BC	SUBURBAN	+	+	+
Trafford	Trafford Metropolitan BC	URBAN BACKGROUND	+	+	+
Wigan	Wigan Metropolitan BC	URBAN BACKGROUND		+	+
Wokingham Earley	Wokingham DC	ROADSIDE		+	+
Wokingham Winnersh	Wokingham DC	URBAN BACKGROUND			+

Appendix 7: Mathematical justification for the addition of contributions to pollutant concentrations from component emission sources

A number of methods are proposed in this report for the annual audit of contributions to annual average pollutant concentrations from sources regulated by the Environment Agency.

The methods generally make use of a time-averaged footprint (or kernel) representing the source-receptor relationship between a certain category of source and locations near to that source. The total annual mean concentration is then calculated as the sum of the contributions from each source or source category. This kernel-based approach considerably simplifies the audit process. This appendix provides the mathematical justification for the methods used.

Mass balance

Consider a volume element in the atmosphere, where gases containing a pollutant A are flowing into the element. A mass balance on the component A leads to the following differential equation:

$$u_x \frac{\partial c_A}{\partial x} + u_y \frac{\partial c_A}{\partial y} + u_z \frac{\partial c_A}{\partial z} + \frac{\partial c_A}{\partial \theta} + c_A \left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \right) - D_{AB} \left(\frac{\partial^2 c_A}{\partial x^2} + \frac{\partial^2 c_A}{\partial y^2} + \frac{\partial^2 c_A}{\partial z^2} \right) + \Lambda_A c_A - R_A = 0$$

where

> u_x, u_y, and u_z are the wind speeds in the x and y horizontal dimension and z vertical dimension;
> c_A is the concentration of A;
> D_{AB} is the molecular diffusivity of A through medium B;
> Λ_A is the wet scavenging coefficient;
> R_A is the rate of production of A by chemical reaction;
> θ is time.

This differential equation is simplified in various ways in most dispersion models. For example, various simplifications are made in order account of atmospheric turbulence. The following discussion is generally applicable to all dispersion models.

Consider the special cases where:

$$R_A = 0$$

$$or$$

$$R_A = -kc_A$$

where k is a reaction rate constant.

These special cases correspond to the case of no chemical reaction or a first order reaction of component A.

The differential equation is now both linear and homogeneous, taking the form:

$$P\frac{\partial c_A}{\partial x}+Q\frac{\partial c_A}{\partial y}+R\frac{\partial c_A}{\partial z}+\frac{\partial c_A}{\partial \theta}+Sc_A-D_{AB}\left(\frac{\partial^2 c_A}{\partial x^2}+\frac{\partial^2 c_A}{\partial y^2}+\frac{\partial^2 c_A}{\partial z^2}\right)=0$$

where P, Q, R and S are functions of x, y, z and θ but are not functions of the concentration.

Each of the terms in the equation is of the first degree in the dependent variable and its partial derivatives: that is, the equation is linear. Each of the terms contains either the dependent variable or one of its derivatives: the equation is homogeneous.

The equation will depart from linearity if the wet scavenging coefficient is dependent on the pollutant concentration. This may be the case, for example, if the rain droplets become saturated or there are complex chemical reactions within the droplets. However, most dispersion models currently used do not take the concentration dependence of the wet scavenging coefficient into account.

Superposition theorem

Assume that c_{A1} and c_{A2} are particular solutions of the differential equation corresponding to emissions resulting from source 1 and source 2. The following superposition theorem holds for linear homogeneous differential equations (Kreyszig).

If c_{A1} and c_{A2} are any solutions of a linear homogeneous partial differential equation in some region, then

$$c_A = a_1 c_{A1} + a_2 c_{A2}$$

is also a solution of that equation in that region, where a_1 and a_2 are any constants (including unity).

Proof of the theorem is obtained by substitution,

More generally, by extension for i sources

$$c_A = \sum_i a_i c_{Ai}$$

is also a solution of the differential equation, if c_{Ai} are particular solutions of the differential equation corresponding to emissions sources i.

It follows then that the concentrations at a particular point in space and time may be calculated as the sum of the contributions from individual sources, provided the differential equation is both linear and homogeneous.

It also follows that if the c_{Ai} are determined for unit emission from each source, then the constants a_i will correspond to the rates of emission. The kernel approach applies the superposition theorem in this way.

It is important to note that the superposition theorem does not hold in general for non-homogeneous or non-linear partial differential equations. Thus, the method will be in error if the rate of reaction is neither zero nor represented by a first order reaction. However, the error may be small if the reaction rate is small or can be approximated by a first order reaction over a limited range.

The case where the reaction rate, R_A , is specified as a function of time and space is a special non-homogeneous case. The mass balance differential equation is then represented by:

$$f(x,y,z,\theta) = P\frac{\partial c_A}{\partial x} + Q\frac{\partial c_A}{\partial y} + R\frac{\partial c_A}{\partial z} + \frac{\partial c_A}{\partial \theta} + Sc_A - D_{AB}\left(\frac{\partial^2 c_A}{\partial x^2} + \frac{\partial^2 c_A}{\partial y^2} + \frac{\partial^2 c_A}{\partial z^2}\right) = U$$

where U is a function of x,y,z and time but not a function of the pollutant concentration.

It is readily seen that if c_{A1} is a solution of this equation (equation B) and c_{A2} is a solution of the characteristic equation (that is, the differential equation with U=0, equation A), then $c_{A1}+c_{A2}$ is also a solution of the mass balance differential equation, B.

By means of this result, it is possible to combine general solutions of the characteristic equation A with particular integrals B of the above equation to achieve general solutions of B. Note also that if c_{A1} and c_{A2} are solutions of $f=U_1$ and $f=U_2$ respectively, then $c_{A1}+c_{A2}$ is a solution of $f=U_1+U_2$. This means that if a pollutant is formed as the result of first order chemical reactions of a precursor species emitted from several sources, then it is possible to add the contributions from each of the sources. For example, if sulphur dioxide is emitted from a number of sources and reacts with a first order reaction in the atmosphere to create sulphate aerosol, then the concentration of the sulphate aerosol may be calculated as the sum of contributions from each of the sulphur dioxide sources.

It is also necessary that the boundary conditions applied meet the superposition principle. Thus, it should be possible to represent the solution of the differential equation at the boundary by a linear sum of component solutions. For most boundary conditions, for example those of the forms c_A=constant, $c_A=0$, dc_A/dx=constant, $dc_A/dx=0$ or $d^2c_A/dx^2=0$, this is the case. It is also possible to represent the solution at the boundary as a linear sum of component solutions for the dry deposition case:

$$\frac{c_A}{r_s} + D_A\frac{\partial c_A}{\partial z} = 0$$

where r_s is the surface resistance below the laminar sublayer.

The case where there is an equilibrium surface concentration (compensation point) may also be represented in terms of a linear sum of component solutions.

There are some cases where the surface resistance depends on the pollutant concentration. For example, the surface may become saturated with the pollutant or there may be complex chemical reactions at the surface. It will not then be possible to represent the solution at the boundary as the linear sum of component solutions. Complex surface resistance models have been suggested for some pollutants and have been included in the EMEP unified model. However, they are not well-established and have not been more generally applied.

Average concentrations

The differential equation representing the mass balance on the pollutant and the solution of the equation apply for short periods during which the air velocity and boundary conditions remain effectively constant. Under turbulent atmospheric conditions, the velocity field is changing rapidly and so the concentration will also change rapidly. The annual audit is based on an assessment of time-averaged concentrations. Most dispersion models apply some approximations to take account of the turbulent fluctuations in air velocity and concentrations. For example, many dispersion models calculate hourly average concentrations. The basic principle set out below remains the same, however. The time-average concentration is given by:

$$c_{Aaverage} = \frac{\sum_{N} c_{An}}{N}$$

where c_{An} is the total concentration during time increment, n, and N is the total number of time increments during the averaging time.

For the case where many sources contribute to the total concentration, the time average concentration is:

$$c_{Aaverage} = \frac{\sum_{N}\left(\sum_{i} c_{Ain}\right)}{N}$$

Applying the commutative and associative laws of addition, this may be rewritten as:

$$c_{Aaverage} = \frac{\sum_{i}\left(\sum_{N} c_{Ain}\right)}{N}$$

This means that the sum of the time-averaged contributions from each source is exactly equivalent to the time-averaged sum of the contributions. The kernel approach used in the proposed annual audit method makes use of this identity.

Summary

The kernel approach used in the proposed annual audit method relies on the theorem of superposition and the commutative and associative laws of addition. The superposition theorem applies for linear homogeneous partial differential equations only and this limits the application of the method to the case when rates of chemical reaction of the pollutant are small or are represented, at least approximately, by first order chemical kinetics. The method may also be inappropriate where the surface resistance to dry deposition or the wet scavenging coefficient are dependent on pollutant concentrations.

In practice, the method uses the dispersion model ADMS 3 as an approximation to the differential equation representing the mass balance of the pollutants. The model relies on meteorological data with limited spatial resolution. Use of the kernel approach implies that the meteorological data used to prepare the kernel apply throughout its area of application. Spatial analysis of meteorological data presented in Appendix 4 suggests that the error introduced is small.

Appendix 8: Sector average emissions calculations in TRACK

TRACK Versions 1.6d onwards eliminate the star patterns seen in earlier versions around major point sources. It averages the emissions along a tangent to the trajectory across the wind direction segment at each point on the trajectory instead of using a nearest neighbour approach.

Suppose that the trajectory is at Δx, Δy with respect to the receptor at x_0, y_0. Also assume that there are n wind angle sectors. Version 1.6d averages emissions along the tangent from

$$\begin{aligned} x_1 &= x_0 + \Delta x - \Delta y \tan(\pi / n) \\ y_1 &= y_0 + \Delta y + \Delta x \tan(\pi / n) \end{aligned}$$

to

$$\begin{aligned} x_2 &= x_0 + \Delta x + \Delta y \tan(\pi / n) \\ y_2 &= y_0 + \Delta y - \Delta x \tan(\pi / n) \end{aligned}$$

The average is calculated using the trapezium rule with dl = l/20.

The change has a very small effect on national average predicted concentrations due to rounding/integration errors. This effect may be shown by comparing predicted concentrations for the base model year run using Version 1.6d and Version 1.6c, which were in other ways identical. The predicted average concentrations for 2003 over 833 receptors on a 20 km Cartesian grid covering the land area of the UK for runs base_02_6c_vg4 and base_02_6d_vg4 are given in Table A8.1:

Table 8.1: Predicted average concentrations for 2003 over UK land area on a 20 km Cartesian grid

Species	**Concentration, μg m^{-3}**	
	1.6c	**1.6d**
NO_x	5.45	5.37
NO_2	4.09	4.04
HNO_3	0.04	0.04
HONO	0.02	0.02
PAN	6.73	6.68
AN	3.57	3.60
ANI	0.07	0.07
SO_2	2.63	2.63
SO_4	0.42	0.41
AS	0.27	0.28
HCl	0.09	0.09

Figures A8.1 and A8.2 show the difference in sulphur dioxide concentrations in μg m^{-3} between Versions 6d and 6c. The effect of the model change is shown most clearly in Figure A8.2, which shows alternatively positive and negative changes in concentrations across the width of Scotland on sectors centred on the English power stations in the Aire and Trent valleys.

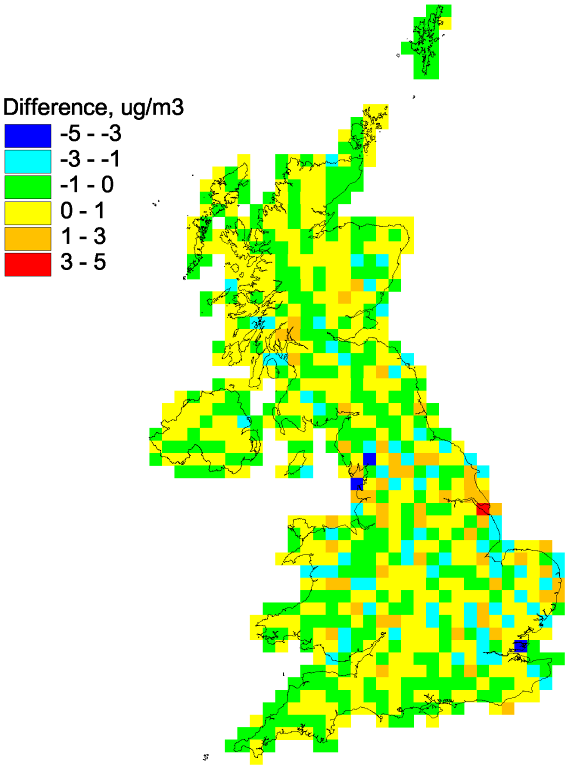


Figure A8.1: Differences in sulphur dioxide concentration between Version c and Version d of TRACK model (μg m^{-3}) using a fine difference scale

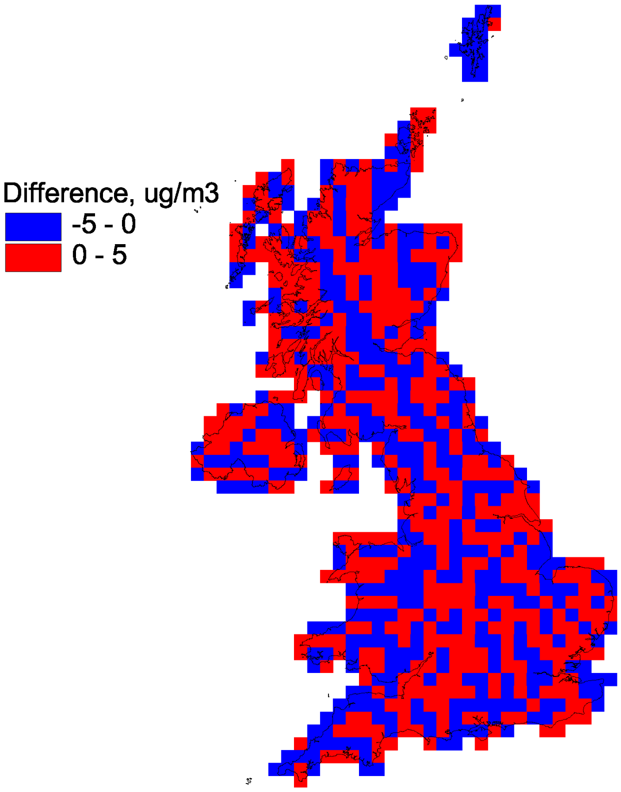


Figure A8.2: Differences in sulphur dioxide concentration between Version c and Version d of TRACK model (μg m^{-3}) using a coarse difference scale

Appendix 9: Surface resistance to dry deposition of sulphur dioxide

Consider a thin film of water covering the surface of the ground and vegetation. The partial pressures of sulphur dioxide and ammonia in the water film at the interface are in equilibrium with the gas above it. The concentrations of sulphur dioxide and ammonia in the liquid may be estimated using Henry's law:

$$[NH_3] = H_{NH3} p_{NH3}$$
$$[SO_2] = H_{SO2} p_{SO2}$$

where

[] are the concentrations in moles l^{-1};
H_{NH3} is the Henry's law constant for ammonia, 62 mol $l^{-1}atm^{-1}$;
H_{SO2} is the Henry's law constant for sulphur dioxide, 1.2 mol $l^{-1}atm^{-1}$;
p_{NH3} and p_{SO2} are the partial pressures of ammonia and sulphur dioxide.

Sulphur dioxide dissociates in water primarily to the bisulphite ion: at pH less than 4, dissociation to the sulphite ion becomes significant, but is ignored here.

$$[HSO_3^-] = \frac{K_{SO2}[SO_2]}{[H^+]}$$

Similarly, ammonia dissociates to form the ammonium ion:

$$[NH_4^+] = \frac{K_{NH3}[NH_3]}{[OH^-]}$$

where K_{SO2} and K_{NH3} are equilibrium constants 0.0132 and 1.7 x 10^{-5} respectively.

The OH^- and H^+ concentrations are related by the dissociation constant of water:

$$[OH^-][H^+] = K_w = 10^{-14}$$

The solution is electrically neutral:

$$[H^+] + [NH_4^+] = [OH^-] + [HSO_3^-]$$

Rearranging for $[H^+]$:

$$[H^+] = \sqrt{\frac{K_w(K_w + H_{SO2}K_{SO2}p_{SO2})}{(K_w + H_{NH3}K_{NH3}p_{NH3})}}$$

The concentrations of the other species in solution may then be obtained by substitution.

The bisulphite ion and other ions diffuse from the interface into the body of the liquid film. The average liquid-side mass transfer coefficient k_{Lav} is given by penetration theory:

$$k_{Lav} = 2\sqrt{\frac{D_{AB}}{\pi\theta}}$$

where D_{AB} is the diffusion coefficient of the bisulphite ion in water, taken to be 1.9×10^{-5} m^2 s^{-1} (an equivalent ionic conductivity of 70 ohm^{-1} cm^2 $equiv^{-1}$). θ is the penetration time corresponding to the time since the water surface was created. It was assumed that a new surface was created every 24 hours with each dew fall.

This may be converted into an equivalent gas-side surface resistance:

$$R_c = \frac{[H^+]}{(1000H_{SO2})K_{SO2}k_{Lav}RT}$$

where R is the gas constant, 8.205×10^{-5} m^3 atm K^{-1} $mole^{-1}$, and T is the ambient temperature, 298 K. The 1000 factor converts Henry's law constant to moles m^{-3} atm^{-1}.

The surface resistance has been evaluated for a range of interface sulphur dioxide (1-100 ppb) and ammonia (0.5-2 ppb) concentrations (Figure A9.1)

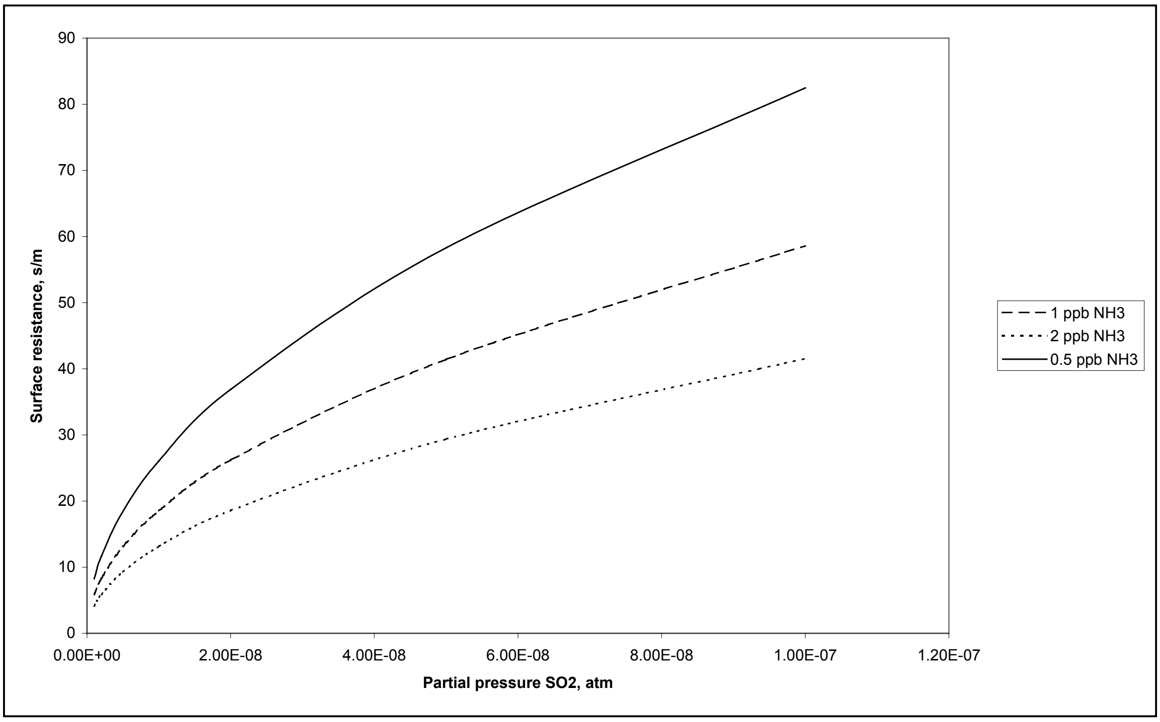


Fig. A9.1: Surface resistance dependence on ammonia and sulphur dioxide concentrations

We are The Environment Agency. It's our job to look after your environment and make it **a better place** – for you, and for future generations.

Your environment is the air you breathe, the water you drink and the ground you walk on. Working with business, Government and society as a whole, we are making your environment cleaner and healthier.

The Environment Agency. Out there, making your environment a better place.

Published by:

Environment Agency
Rio House
Waterside Drive, Aztec West
Almondsbury, Bristol BS32 4UD
Tel: 0870 8506506
Email: enquiries@environment-agency.gov.uk
www.environment-agency.gov.uk