

Evidence

Comparison of simple and advanced regional models (CREMO)

Model Evaluation Protocol

Report – SC060037/a

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Miranda Kavanagh

Director of Evidence

Executive summary

The Environment Agency is responsible for the regulation of specific industrial sectors and has long used regional-scale atmospheric chemical transport models to assist in setting emission limits. The Department for Environment, Food and Rural Affairs (Defra) also makes use of such models to assist in the development of policy measures relating to the environmental impacts resulting from such emissions. Defra and the Environment Agency have used a number of different models to cover specific impacts and spatial scales. Since the late 1990s, a number of ‘advanced’ models have been developed with the capability to address multi-pollutant issues on multiple scales. One of these advanced models is the Community Multiscale Air Quality (CMAQ) modelling system developed originally by the US Environmental Protection Agency.

The overall aim of the ‘Comparison of simple and advanced regional models’ (CREMO) project was to enable the Environment Agency to make an informed decision on the use of advanced regional-scale atmospheric chemical transport models as an assessment tool. In particular, the project evaluated the performance characteristics of advanced regional air quality models for real regulatory applications through comparison of CMAQ with existing methods. The project applied CMAQ to a series of assessments (including acid deposition, particulate matter and ozone) and test its capabilities through targeted comparisons with ‘simpler’ models and with measurements according to agreed model acceptance criteria.

The main models used in the CREMO project are the:

- CMAQ modelling system, operated in the UK by the University of Hertfordshire and the UK power generators;
- FRAME (Fine Resolution Atmospheric Multi-pollutant Exchange) model, developed and operated by the Centre for Ecology and Hydrology (CEH);
- TRACK-ADMS (Trajectory model with Atmospheric Chemical Kinetics–Atmospheric Dispersion Modelling System), developed and operated by AEA Technology
- OSRM (Ozone Source–Receptor Model), developed and operated by AEA Technology.

Model evaluation is a key part of the iterative cycle of model development, testing and confidence building. An important goal of the performance evaluation is to:

- determine a model’s degree of acceptability and usefulness for a specified task;
- establish that the model is providing the results for the right reasons.

This report sets out the protocol for the evaluations and model intercomparisons in the CREMO project. It provides a brief description of the models used, details of the protocol and how they were applied. The tasks proposed for the CREMO project enabled operational, dynamic and diagnostic evaluations of the models and their performances. As a first step to understanding commonalities and differences between the models, information has been compiled on the structure of the models, the treatment of different physical and chemical processes, input data, computational requirements, *etc.* to demonstrate that the model is based on generally accepted science and computational methods. All the models have been subject to scientific peer review. The Defra Model Evaluation Exercise provides additional information on the models’ performance.

Operational evaluation involves comparison of modelled outputs against the observed quantity (or parameter derived from observations). For the CREMO project, this comparison was based on model runs undertaken for a UK domain for the 2003 calendar year, which was a particularly warm and photochemically active year with a major ozone episode in August.

Dynamic evaluation considers the response of the model to changes in meteorology and/or emissions. Two types of dynamic evaluation were undertaken in the CREMO project:

- identification of a period in 2003 when there was a significant change in meteorology;
- comparison of the model responses (footprints) arising from emission changes from two facilities (a power station and an oil refinery) regulated by the Environment Agency.

A diagnostic evaluation is designed to assess the adequacy of the treatment of physical and chemical processes in the model. One of the key elements of regional air quality models, especially for ground-level ozone, is the chemical mechanism. Different chemical mechanisms are used in the models in the CREMO project. As part of the CREMO project, the carbon-bond mechanism (CBM) and OSRM chemical mechanisms were compared with a set of other widely used chemical mechanisms, including the Master Chemical Mechanism (MCM) and its derived mechanism Common Representative Intermediates (CRI). The Master Chemical Mechanism is considered to represent the current state of knowledge and is taken as the reference mechanism for the comparison.

Various acceptance criteria exist based on expert judgement following analysis of actual performance. The report considers the criteria specified in the USA and in the EU Air Quality Directive together with the criteria recommended for the Defra model evaluation protocol. It concludes that the parameters used in the Defra model intercomparison define the minimum acceptable level of model performance:

- The fraction of modelled concentration or metric that lie within ± 50 per cent of the observed value should be greater than 50 per cent.
- The normalised mean bias (*NMB*) should be $-0.2 \leq NMB \leq 0.2$.

The CREMO project has generated some valuable input data sets and model outputs. It is recommended that these should become a benchmark dataset and made available to the air quality modelling community.

The model evaluation and the outcomes of the CREMO project are detailed in the reports.

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1 Introduction

The overall aim of the ‘Comparison of simple and advanced regional models’ (CREMO) project was to enable the Environment Agency to make an informed decision on the use of advanced regional-scale atmospheric chemical transport models as one of its assessment tools. In particular the project evaluated the performance characteristics of the Community Multiscale Air Quality (CMAQ) modelling system¹ for real regulatory applications through comparison of CMAQ with existing methods. The project applied CMAQ to a series of assessments (including acid deposition, particulate matter and ozone) and tested its capabilities through targeted comparisons with ‘simpler’ models and with measurements according to agreed model acceptance criteria.

1.1 Background

The emissions of sulphur dioxide (SO₂), oxides of nitrogen (NO_x), volatile organic compounds (VOCs) and ammonia contribute to a number of environmental impacts which affect human health and/or ecosystems:

- acid deposition/eutrophication;
- ground-level ozone;
- particulate matter (PM).

These impacts do not necessarily occur in the immediate vicinity of the emission source but often involve long-range transport to the affected areas, a result of the timescales for chemical processing of the emissions in the atmosphere.

In recognition of this, policy options and control measures have been agreed internationally through:

- protocols to the UNECE Convention on Long-range Transboundary Air Pollution (CLRTAP) (for example, the Gothenburg Protocol);
- European Union Directives, especially the National Emission Ceilings Directive, the Large Combustion Plant Directive, the Directive on Integrated Pollution Prevention and Control (IPPC) and the Habitats Directive.

In the UK, the Environment Agency is responsible for the regulation of specific industrial sectors and has long used regional-scale atmospheric chemical transport models to assist in setting emission limits. The Department for Environment, Food and Rural Affairs (Defra) also makes use of such models to assist in the development of policy measures relating to the environmental impacts resulting from such emissions, including provision of input into the United Nations Economic Commission for Europe (UNECE) CLRTAP protocols and EU Directives.

¹ When the project was commissioned, MODELS-3 was the operational version of this community air quality model. MODELS-3 comprised the CMAQ modelling system and the MM5 mesoscale meteorological model. The MM5 model has since been replaced by the Weather Research and Forecasting (WRF) numerical weather prediction model. All references to MODELS-3 have been updated to CMAQ to avoid confusion.

A number of different models have been used by Defra and the Environment Agency to cover specific impacts and spatial scales such as:

- Fine Resolution Atmosphere Multi-Pollutant Exchange (FRAME) for acid deposition;
- The Trajectory model with Atmospheric Chemical Kinetics–Atmospheric Dispersion Modelling System (TRACK-ADMS) for annual audits;
- the Ozone Source–Receptor Model (OSRM) for ozone.

Since the late 1990s, a number of ‘advanced’ models have been developed with the capability to address multi-pollutant issues on multiple scales. These modelling systems include the:

- Community Multiscale Air Quality (CMAQ) modelling system (Byun and Schere 2006);
- Unified European Monitoring and Evaluation Programme (EMEP) model (Simpson *et al.* 2003);
- CHIMERE model (Bessagnet *et al.* 2009 and references therein).

These are all available for use by the air pollution research community.

In 2007 Defra commissioned a review of its ozone modelling tools (including OSRM) (Monks *et al.* 2007) as part of a wider review of its air pollution modelling activities. The review noted that the UK modelling approach differed from other countries in its use of boundary layer trajectory models. One of its key recommendations (R1.1) was to move to a Eulerian framework as used by advanced models such as CMAQ and EMEP. Other recommendations were to:

- compare Eulerian model results with the results from observations and with those from comparative Lagrangian models to ensure continuity (R 1.2);
- conduct a model comparison exercise where two of the current Lagrangian-based models are compared to two (or more) regional air quality Eulerian-based models.

As part of the Joint Environment Programme (JEP), the power generators (E.ON and RWE npower) have been using CMAQ to investigate the contribution and significance of the power generation sector (see, for example, Griffiths and Lennard 2006, Lennard *et al.* 2006, Sutton 2008).

1.2 Project aims and objectives

The CREMO project has two main aims:

1. To provide a technique for assessing the contribution of industrial emissions of NO_x and VOCs under realistic meteorological conditions to ambient levels of ozone based on CMAQ and involving comparison with simpler methods and observations.
2. To provide a technique for assessing the contribution of industrial emissions under realistic meteorological conditions to ambient levels of PM₁₀ and PM_{2.5}, based on CMAQ and involving comparison with simpler methods and observations.

These aims were met by the following specific objectives:

- To compare the performance of CMAQ with the simpler models, FRAME and TRACK-ADMS, and to produce footprints of deposition and concentrations resulting from industrial emissions regulated by the Environment Agency.

- To assess the capabilities of CMAQ as a practical tool for modelling acid deposition, ozone and size-speciated particulate matter;
- To evaluate the capabilities of CMAQ to predict regional ozone concentrations and their response to changes in emissions of NO_x and VOCs.
- To assess the capabilities of CMAQ to calculate the contribution of regulated industrial emissions to size-speciated particulate matter concentrations and associated chemical species.
- To identify the main operational applications of CMAQ by examining the variability and uncertainty resulting from changes to input parameters through sensitivity analysis.
- To synthesise and integrate the outcomes of previous tasks and make recommendations on how and under what circumstances CMAQ should be used by the Environment Agency for regulatory applications.

1.3 Structure of report

This report describes the model evaluation protocol developed for the CREMO project. It updates and extends an earlier version prepared by Yu *et al.* (2007). Section 2 provides a brief description of the models used in the CREMO project while Section 3 defines the model evaluation protocol and how it is applied. Section 4 reviews model acceptance and discusses acceptance criteria. Conclusions and recommendations are set out in Section 5.

2 Description of the models

The following sections provide brief details of each of the main models in the CREMO project. These models are:

- CMAQ modelling system, operated by the University of Hertfordshire and the power generators;
- FRAME model, developed and operated by the Centre for Ecology and Hydrology (CEH);
- TRACK-ADMS, developed and operated by AEA Technology;
- OSRM, developed and operated by AEA Technology.

Appendix 1 provides further information on key features of the different models including treatment of meteorology, chemical schemes, deposition and emissions.

2.1 Community Multiscale Air Quality modelling system

The Community Multiscale Air Quality (CMAQ) modelling system is a comprehensive modelling system developed by the US Environmental Protection Agency (USEPA). As MODELS-3, it consisted of the MM5 meteorological model and the CMAQ photochemical model.

CMAQ is a Eulerian photochemical air quality model based on the 'one atmosphere' concept where complex interactions between atmospheric pollutants on urban, regional and hemispheric scales are treated in a consistent framework. It is designed for assessing the impact of multiple pollutants including tropospheric O₃ and other oxidants, aerosols and acid deposition.

The CMAQ modelling system is able to process large amount of diverse information from complicated emission mixtures to complex distribution of sources. It can also simulate the complex atmospheric processes that transport and transform these pollutants in a dynamic environment that operates in a large range of timescales covering minutes to days and weeks. The corresponding spatial scales covered are commensurately large, ranging from urban to continental scales. CMAQ is an open-source, community-supported model with many of its components, including chemistry schemes, chemistry solvers and numerical schemes, being updated with the latest outcomes from the research community.

From version 4.5, CMAQ has incorporated sulphate tracking capability and primary carbon source apportionment capability. The sulphate tracking diagnostic model configuration can explicitly track the separate contributions to sulphate from the gas phase and five aqueous phase chemical reactions, as well as contributions from direct emissions and initial and boundary conditions. The primary carbon source diagnostic model configuration can provide detailed information on the source origin of primary carbonaceous aerosol and track the contributions of elemental carbon and primary organic carbon from 10 different source categories or source regions.

In version 4.6, the CB-IV chemical mechanism (Gery *et al.* 1989) was replaced with the CB05 mechanism (Yarwood *et al.* 2005). The CB05 mechanism has an improved treatment of the formation of secondary organic aerosols (SOAs). Inorganic reactions were also updated to account better for the range of conditions of temperature, pressure and chemical environment encountered in annual simulations at scales ranging from urban to continental.

The tri-modal approach to aerosol size distribution based on that in the Regional Particulate Model (RPM) (Binkowski and Shankar 1995), which discriminates PM into coarse PM and speciated PM_{2.5} (that is PM smaller than 2.5 µm aerodynamic diameter), was used in order to model PM (see Binkowski and Roselle 2003). The subspecies considered are sulphate (SO₄²⁻), nitrate (NO₃⁻), ammonium (NH₄⁺), sodium (Na⁺), chloride (Cl⁻), water (H₂O) and organics from precursors of anthropogenic and biogenic origin. Each mode (Aitken, accumulation and coarse) is subjected to both wet and dry deposition.

The Weather Research and Forecasting (WRF) model is now used as the meteorological driver for the CMAQ modelling system. The Meteorology–Chemistry Interface Processor (known as MCIP) version 3.4.1 (Otte and Pleim 2010) was used to translate WRF meteorological data to the format required by CMAQ.

More detailed descriptions of CMAQ including its theoretical formulations, chemical and physical process parameterisations, numerical algorithms and complete mechanism listings can be found in Byun and Ching (1999) and Byun and Schere (2006). Additional and updated documentation is available from the official CMAQ website (<http://www.cmaq-model.org>). Developments and improvements were made during the project lifetime.

2.2 FRAME

The FRAME (Fine Resolution Atmospheric Multi-pollutant Exchange) model is a Lagrangian atmospheric transport model used to assess the long-term annual mean deposition of reduced and oxidised nitrogen and sulphur over the UK.

A detailed description of the FRAME model is contained in Singles *et al.* (1998). Fournier *et al.* (2002) described the development of a parallelised version of the model with an extended domain that includes Northern Ireland and the Republic of Ireland. The model was developed from an earlier European scale model, Transport over Europe of Reduced Nitrogen (TERN) (ApSimon *et al.* 1994).

FRAME was developed initially to focus in particular on the transport and deposition of reduced nitrogen and was named the Fine Resolution AMmonia Exchange model. Recent developments in the treatment of sulphur and oxidised nitrogen (Fournier *et al.* 2004) mean that it may now be considered a robust multi-chemical species tool. The new name reflects these changes while preserving the familiar acronym. Recent publications on the FRAME model include Dore *et al.* (2007), Matejko *et al.* (2009) and Vieno *et al.* (2010).

2.3 TRACK-ADMS

AEA Technology developed the nested modelling system, TRACK-ADMS, to produce high-resolution maps of the concentrations and rates of deposition of acidifying and eutrophying species and base cations across the UK. TRACK-ADMS has been used in recent work for the Environment Agency to assess the contribution of processes regulated by the Environment Agency (for England and Wales) and the Scottish Environment Protection Agency (SEPA) to national concentrations and deposition budgets (Abbott and Vincent 2006). TRACK-ADMS built on AEA Technology's modelling work for the Environment Agency and Defra's Pollution Climate Mapping contract.

TRACK-ADMS consists of two main components:

- The Lagrangian atmospheric transport model TRACK (Lee *et al.* 1999a, b) is used to calculate the contributions to each receptor from emission sources more than 50 km

from the receptor. The contributions from these more distant sources is calculated on a lower resolution (10–20 km grid), which is then interpolated onto the 1 km receptor grid.

- The dispersion model ADMS 3.3 is used to calculate the contributions to each receptor from industrial point sources and area sources less than 50 km from the receptor location. ADMS 3.3 is an up-to-date model of dispersion in the atmosphere of passive, buoyant or slightly dense, continuous or finite duration releases from single or multiple sources.

2.4 Ozone Source–Receptor Model

The Ozone Source–Receptor Model (OSRM) is a recently developed model to describe photochemical ozone production in the UK (Hayman *et al.* 2010). It is one of the tools used by Defra to assist in the development of policy on ground-level ozone.

OSRM covers the EMEP model domain and uses meteorological data sets provided by the UK Met Office to derive 96-hour back trajectories to specified receptor sites (UK/EMEP monitoring sites or a 10km × 10km grid covering the UK). The chemical scheme has been modified from that used in the STOCHEM model (Collins *et al.* 1997, 2000). The mechanism represents ozone formation using 10 VOCs which provides an appropriate description of ozone formation on a regional scale. The emission inventories are taken from EMEP for Europe with the option to use National Atmospheric Emissions Inventory (NAEI) emission inventories for the UK, which have been aggregated to 10 km × 10 km and into eight key sectors.

OSRM is similar in concept to the UK Photochemical Trajectory Model (PTM) (Derwent *et al.* 1998, 2004) in that it simulates the chemical development of species in an air parcel moving along a trajectory and to the ELMO source–receptor model developed by the Universities of Edinburgh/Lancaster and the UK Met Office (Metcalf *et al.* 2002) in that calculations can be undertaken to a 10 km × 10 km grid covering the UK. However OSRM has a number of notable enhancements and advantages to these models.

2.5 UK Photochemical Trajectory Model

The UK Photochemical Trajectory Model (PTM) is a boundary-layer Lagrangian trajectory model for ground-level ozone that has long been used for policy applications (Derwent *et al.* 1998, 2004, 2007). One advantage of the Lagrangian framework in the PTM is the capability to include large comprehensive chemical mechanisms such as the Master Chemical Mechanism (MCM). PTM, OSRM (Hayman *et al.* 2010) and the ELMO model (Metcalf *et al.* 2002) share many common features.

A key application of PTM has been to derive photochemical ozone creation potentials (POCPs) to rank VOCs according to their ability to form ozone. The POCP is derived by considering a relative change in ozone to a change in emissions of each VOC, in turn, integrated over the entire trajectory path under fixed, but representative meteorological conditions. This is used to obtain the change in ozone production for each VOC compared with the change in ozone production for ethylene (ethene), taken to be the reference compound. Other examples can be found in Hayman and Derwent (1997) and Jenkin and Hayman (1999).

A related approach, the integrated downwind ozone production, IDOP, enables the comparison of two VOC species, or two emission sources, in terms of how much ozone is

produced in the downwind environment under ideal conditions (Derwent and Nelson 2003). Further details on the POCP approach can be found in Derwent *et al.* (1998).

3 Model evaluation protocol

3.1 Introduction

Because air pollution models (and environmental models more generally) are widely used in regulatory and decision-making applications, there has been much literature, especially in the USA, about the meaning and use of terms such as verification, validation and evaluation (see Box 3.1). The term 'model evaluation' is now used to demonstrate that a model is suitable for its intended application.

Box 3.1 Model evaluation, validation and verification

Oreskes *et al.* (1994) defined verification and validation as follows:

Verification means to assert or establish truth. A model is said to be verified if its truth has been demonstrated. It is not possible to demonstrate the truth of any proposition except in a closed system.

Validation does not necessarily denote the establishment of truth. Rather, it denotes the establishment of legitimacy. A model that does not contain known or detectable flaws and is internally consistent can be said to be valid.

They argued from a philosophical perspective that a complex computational model can never be truly validated, only invalidated. This is because it is an open system and there are often more parameters that need to be specified than there are available data.

The US National Research Council (NRC 2007) described the key elements of model evaluation in its report on the requirements of environmental models for regulatory applications. The report considered model evaluation to be an ongoing process and identified the following key questions (taken from Beck 2002):

1. Is the model based on generally accepted science and computational methods?
2. Does it work, that is, does it fulfil its designated task or serve its intended purpose?
3. Does its behaviour approximate that observed in the system being modelled?

The USEPA* has developed a framework to describe the different aspects of model evaluation for air quality applications (see also Dennis *et al.* 2010):

- i. **Operational evaluation** is a comparison of model-predicted and routinely measured concentrations of the end-point pollutant(s) of interest in an overall sense. This is the first phase of any model evaluation study.
- ii. **Diagnostic evaluation** entails investigating the atmospheric processes and input drivers that affect model performance to guide model development and improvements needed in emissions and meteorological data.
- iii. **Dynamic evaluation** assesses a model's air quality response to changes in meteorology or emissions, which is a principal use of an air quality model for air quality management.
- iv. **Probabilistic evaluation** strives to characterise uncertainty of the model predictions for model applications such as predicted concentration changes in response to emission reductions

Since these four types of model evaluation are not necessarily mutually exclusive, research studies often incorporate aspects from more than one category of evaluation.

* <http://www.epa.gov/AMD/index.html>

In the CREMO project and following Box 3.1, the proposed tasks initiate operational, dynamic and diagnostic evaluations of the models and their performances. As a first step to understanding commonalities and differences between the models, information has been compiled on the structure of the models, the treatment of different physical and chemical processes, input data, computational requirements, *etc.* to demonstrate that the model is based on generally accepted science and computational methods.

3.2 Model descriptions

A template has been prepared to gather basic information on the models being used in the CREMO project (see Appendix A1.1). Templates have been completed for the models described in Section 2 and Table 3.1 provides an overview of their key features.

All the models have been subject to scientific peer review. In addition the modelling teams are involved in the Defra Model Evaluation Exercise, which provides additional information on the performance of these models.

Table 3.1 Overview of the models in the CREMO project

Model	Type of model	References
CMAQ	<u>Description:</u> <ul style="list-style-type: none"> Eulerian, multi-scale multi-pollutant <u>Application:</u> <ul style="list-style-type: none"> Urban to regional scale SO₂, NO_x, O₃, PM, deposition Research and policy model in USA 	Byun and Ching (1999) Byun and Schere (2006) Chemel et al. (2010)
FRAME	<u>Description:</u> <ul style="list-style-type: none"> Lagrangian Multi-pollutant <u>Application:</u> <ul style="list-style-type: none"> Long-term annual mean deposition of reduced and oxidised nitrogen and sulphur 	Dore <i>et al.</i> (2007) Matejko <i>et al.</i> (2009) Vieno <i>et al.</i> (2010)
TRACK-ADMS	<u>Description:</u> <ul style="list-style-type: none"> Lagrangian for TRACK Gaussian for ADMS Multi-pollutant <u>Application:</u> <ul style="list-style-type: none"> Long-term annual mean deposition of reduced and oxidised nitrogen and 	Lee <i>et al.</i> (1999a, b) Abbott and Vincent (2006)

Model	Type of model	References
	sulphur. <ul style="list-style-type: none"> • Annual mean concentration for SO₂, NO₂, sulphate and nitrate aerosol, PM₁₀ • Short-term average concentrations for SO₂ 	
OSRM	<u>Description:</u> <ul style="list-style-type: none"> • Lagrangian trajectory • Ozone and oxides of nitrogen <u>Application:</u> <ul style="list-style-type: none"> • Used as ozone policy model in Defra • Large number of O₃ and NO₂ metrics to assess the effects on human health and vegetation 	Hayman <i>et al.</i> (2010)
UK PTM	<u>Description:</u> <ul style="list-style-type: none"> • Lagrangian trajectory • Ozone and oxides of nitrogen • PM components <u>Application:</u> Urban to regional scale O ₃ and PM	Derwent <i>et al.</i> (1994, 1998, 2007)

3.3 Operational evaluation

Operational evaluation involves a comparison of modelled outputs against the observed quantity (or parameter derived from observations). In the initial phase of the CREMO project in 2007, it was agreed that the comparison would be based on model runs undertaken for a UK domain for the 2003 calendar year. 2003 was selected as this was a particularly warm and photochemically active year with a major ozone episode in August (EEA 2003).

Model configurations and input data

The summary data provided in Tables A1.2 a to d of Appendix A indicate that the models differ significantly in many respects, such as in the treatment of key physical and chemical processes, input data on emissions, meteorology and boundary conditions.

For the CREMO project, it was agreed to harmonise parameters or input data, where practical, as follows:

Meteorological input. The Lagrangian models such as FRAME and TRACK-ADMS use observational data from single or multiple stations as input, while CMAQ uses full four-dimensional meteorological data from meteorological models (WRF and previously MM5). OSRM uses data sets of boundary-layer meteorological parameters generated by the NAME atmospheric pollution dispersion model developed by the Met Office. It was agreed that each model would continue to use its existing treatment of meteorological data.

Chemical mechanism (for ozone). Different chemical mechanisms are used in CMAQ and the OSRM. One purpose of CREMO is to assess whether appropriate chemical schemes are being used (for example for ozone, acid deposition and aerosols). The existing chemical

scheme would be retained in the models but, as part of the project, these were compared (see Section 3.5).

Initial and boundary conditions. Monthly average concentration fields derived from the Met Office's STOCHEM global tropospheric ozone model would be used to provide initial and boundary conditions for CMAQ and OSRM. The usual method of initialisation would be used for the other models

Emissions. All the models use the annual emission estimates from the NAEI for UK emissions and EMEP for non-UK emission sources (see Table 3.2).

Table 3.2 Sources of emission data

Data base	Web address	Resolution	Species
EMEP	http://www.ceip.at/emission-data-webdab/	50 km× 50 km	NO _x , SO ₂ , CO, NH ₃ , NMVOCs, coarse and fine PM by SNAP-1 sectors
EMEP	http://www.ceip.at/emission-data-webdab/	50 km gridded	Volcanic SO _x , DMS
NAEI	http://naei.defra.gov.uk/data_warehouse.php	1 km gridded	NO _x , SO ₂ , CO, NH ₃ , NMVOC, PM ₁₀ by SNAP-1 sectors

Notes: NMVOC = non-methane volatile organic compound

The NAEI covers the UK mainland and Northern Ireland, and is available as a set of annual emissions maps by SNAP level 1 sector at a spatial resolution of 1 km × 1 km. Similarly gridded annual emission inventories are available on the EMEP website for the EMEP domain at SNAP level 1 sector. The spatial resolution is 50 km × 50 km.

Although the same annual emission data sets are used, differences can arise from the temporal and spatial disaggregation of the speciated emissions, as well as the treatment of large stacks. The model intercomparison uses, as far as is possible, the same data sources (for example EMEP, NAEI) and treatment of the emissions.

The CREMO project is mainly interested in sources regulated by the Environment Agency that are classified as large point sources. As the NAEI point source emission inventory does not contain all the information needed to describe these emission sources in air quality models (such as stack parameters), the following were prepared:

- a generic point source emission inventory including published emissions data from the NAEI website but allocated to different SNAP sectors and estimated stack parameters.
- a more detailed point source emissions inventory including hourly profiles for all of the coal and oil-fired power stations for 2003 (prepared by E.ON).

The format for the generic point source emissions inventory is given in Table 3.3. The format for the detailed point source emissions inventory is the Sparse Matrix Operator Kernel Emissions (SMOKE) ready Inventory Data Analyser (IDA) format.

Emission data from the European Pollutant Emission Register (EPER) was not used in this study as large uncertainties exist in this source. Locations of point sources may, however, be used for spatial allocation of EMEP emissions.

For **biogenic emissions**, the existing approaches in the models were retained.

Table 3.3 Format of generic emissions inventory as an example

Parameter	Value
Plant ID	51
Easting	466400
Northing	426400
Operator	AES Drax Power Ltd
SNAP sector	1
Stack height (m)	259
Stack diameter (m)	15.38
Stack gas exit temperature (°C)	90
Stack gas exit velocity (m/s)	30
NO _x (tonnes per year)	49,600
SO ₂ (tonnes per year)	34,800
NH ₃ (tonnes per year)	0
CO (tonnes per year)	8,150
PM ₁₀ (tonnes per year)	242
PM _{2.5} (tonnes per year)	100
VOCs (tonnes per year)	200

Meteorology

Many of the models in the CREMO project use hourly meteorological datasets derived from numerical weather prediction models (for example CMAQ now uses the WRF model (<http://www.wrf-model.org>)). Meteorology is a major determinant of pollutant concentrations as it influences the emission source regions sampled, dispersion and the chemical evolution of air masses. Furthermore meteorological conditions not only impact the dispersion of pollutants but also the chemical transformation processes of pollutants, the intensity of biogenic emissions, and the efficiency of dry and wet removal (GAW 2008).

Available air pollution measurements

The model intercomparison was based on measurements made at UK monitoring sites in 2003. The measurements were taken from the following monitoring networks:

Automatic Urban and Rural Monitoring Network (AURN) This is operated by Defra and the Devolved Administrations, is the main UK monitoring programme and uses automatic instrumentation at sites in rural and urban locations. The species measured at each site include some or all of O₃, NO/NO₂/NO_x, CO, SO₂ and PM₁₀. The monitoring data are available from UK-AIR (<http://uk-air.defra.gov.uk/data/>).

The **UK Acidifying and Eutrophying Atmospheric Pollutants** is a monitoring programme of Defra and the Devolved Administrations. This monitoring programme was formed in 2009 by rationalising a number of separate Defra monitoring networks. The UKEAP programme comprises determination of:

- rainfall and its chemical composition and related species associated are determined at up to 38 rural locations. This was formerly known as the **UK Acid Deposition Monitoring Network (ADMN)**. The monitoring data are also available from UK-AIR;
- acid gases and aerosol components: HNO_3 , NH_3 , SO_2 , HCl , SO_4^{2-} , NO_3^- , Cl^- , Na^+ , Mg^{2+} and Ca^{2+} . This formed the **HNO_3 Denuder and the NH_3 Monitoring Networks** operated by the Centre for Ecology and Hydrology (CEH) for the Department for Environment, Food and Rural Affairs. The network sites are in rural locations and 12 were operational in 2003. The measurements are available from <http://pollutantdeposition.defra.gov.uk/ukeap>.

The monitoring programme operated by the power generators as part of their **Joint Environment Programme (JEP)** provides SO_2 , NO and NO_2 data for sites local to the generators' coal and oil-fired power stations. At a limited number of sites additionally measurements on ozone and PM_{10} are also available.

General information on the species monitored at sites in different UK monitoring networks in 2003 is given in Appendix 2, together with descriptions of the measurement methods. Appendix 3 lists the sites that were operational in 2003 with the species measured at each site.

Model outputs

CMAQ and OSRM can provide output at specified time intervals, typically one hour, which can then be averaged to derive average concentrations over longer periods. The FRAME and TRACK-ADMS models on the other hand generally provide annual mean concentrations. Thus a common set of target parameters was needed for the model comparison and evaluation, taking into account the following considerations:

- standard parameters in operational air quality model validation;
- common output parameters available from all the models;
- parameters important for describing the modelled processes such as deposition;
- ozone chemistry.

The comparison was based on averaging times of relevance to regulatory assessment:

- For deposition (and rainfall), this consisted of annual mean values and annual totals.
- For gas-phase species, this consisted of hourly values and annual averages.
- For particulate species, this consisted of daily (or 24-hour mean) values and annual averages.

Table 3.4 provides an overview of the different parameters selected for model comparison and evaluation, taking account of the available measurements.

Table 3.4 Overview of parameters to be used in the model comparison and evaluation

Parameter	CMAQ	FRAME	TRACK-ADMS	OSRM
Deposition				
SO ₂ (concentration)	H, AM	AM	AM	
NO (concentration)	H, AM	AM	AM	
NO ₂ (concentration)	H, AM	AM	AM	
NO _x (concentration)	H, AM	AM	AM	
NH ₃ (concentration)	H, AM	AM	AM	
HNO ₃ (concentration)	H, M, AM	AM	AM	
Aerosol sulphate (concentration)	H, M, AM	AM	AM	
Aerosol nitrate (concentration)	H, M, AM	AM	AM	
Aerosol ammonium (concentration)	H, M, AM	AM	AM	
Total rainfall amount	AT	AT		
Oxidised S deposition (dry)	AT	AT		
Oxidised N deposition (dry)	AT	AT		
Reduced N deposition (dry)	AT	AT		
Oxidised S deposition (wet)	AT	AT		
Oxidised N deposition (wet)	AT	AT		
Reduced N deposition (wet)	AT	AT		
Dry deposition velocity				
Ozone				
O ₃ concentration	H, AM			H, AM
AOT40	H			H
SOMO35	H			H
NO concentration	H, AM			H, AM
NO ₂ concentration	H, AM			H, AM
NO _x concentration	H, AM			H, AM
Particulate matter				
PM _{2.5} (concentration)	H, AM	AM	AM	
PM ₁₀ (concentration)	H, AM	AM	AM	
Aerosol sulphate (concentration)	H, M, AM	AM	AM	
Aerosol nitrate (concentration)	H, M, AM	AM	AM	
Aerosol ammonium(concentration)	H, M, AM	AM	AM	

Notes: AM = annual mean; AT= annual total; D = daily mean values; H = hourly values; M = monthly averaged values.

Performance statistics/metrics

A variety of statistics have been developed and used over the years to assess the performance of air quality models (see for example Eder *et al.* 2006, Annex E of GAW 2008, Dennis *et al.* 2010). There is no agreed single performance metric to evaluate model performance. Indeed, multiple performance measures should be applied and considered in any model evaluation exercise, as each measure has advantages and disadvantages, and there is no single measure that is universally applicable to all conditions (GAW 2008).

Appendix 4 provides a list of the most commonly used statistical metrics and their definitions. In the CREMO project, the following were derived:

- 1 Accuracy
- 2 Bias
- 3 Correlation coefficient
- 4 Factor of exceedence
- 5 Factor of two
- 6 False alarm ratio
- 7 Fractional bias
- 8 Fractional error
- 9 Hit rate
- 10 Index of agreement
- 11 Fractional bias
- 12 Fractional error
- 13 Mean bias
- 14 Mean error
- 15 Mean normalised bias
- 16 Mean normalised error
- 17 Normalised mean bias
- 18 Root mean square error
- 19 Skill variance

According to the GAW report (2008), the Gaussian distribution based measures, fractional bias (FB) and normalised mean square error (NMSE), may be overly influenced by infrequently occurring high observed and/or predicted concentrations, as the concentration distribution is close to lognormal for most atmospheric pollutants. The correlation coefficient (r) reflects the linear relationship between two variables and is thus insensitive to either an additive or a multiplicative factor. The hit rate is a measure independent of the error distribution. The factor of two (FAC2) is considered to be the most robust measure as it is not overly influenced by outliers.

The metrics listed above should be calculated for each species at each site. It would be useful to derive the metrics for different site types and for different time periods (hours of day, days of week, months of year).

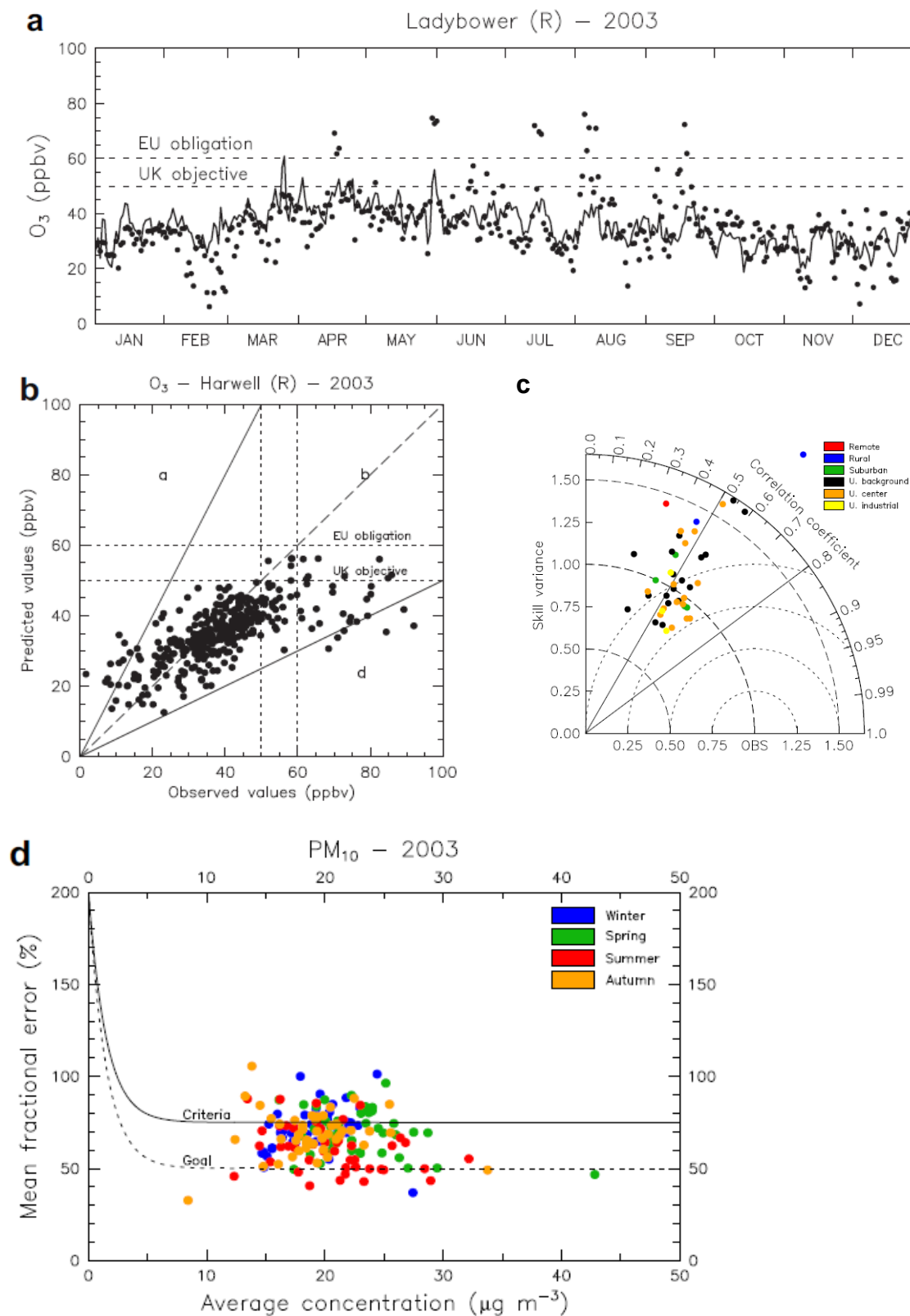


Figure 3.1 Example(a) time series comparison of modelled and observed concentrations, (b) scatter plot of modelled against observed concentrations, (c) Taylor plot and (d) bugle plot (taken from Chemel *et al.* 2010)

Presentation

A variety of methods can be used to compare modelled and measured output. These include time series, scatter plots, Taylor diagrams (Taylor 2001) and 'bugle plots'. Examples of these plots are shown in Figure 3.1. These were applied to the species listed in Table 3.4 to inform the comparisons (Chemel *et al.* 2010).

3.4 Dynamic evaluation

According to the USEPA (see Box 3.1; Dennis *et al.* 2010), a dynamic evaluation considers the response of the model to changes in meteorology and/or emissions, which are of special concern for air quality management.

Within the CREMO project, two types of dynamic evaluation were considered.

1. Identification of periods in 2003 when there were significant changes in meteorology. For example, there were elevated temperatures and ozone concentrations across the southern half of the UK in August 2003. How do the models perform during the episode period compared to the rest of the year?
2. Comparison of the model response arising from emission changes from particular types of industrial facility regulated by the Environment Agency:
 - Case Study A: a large coal-fired power station source. Following a scoping study by the power generators to review local monitoring data, geographical location and 2003 emission totals, it was agreed that this case study should be based on a representative/hypothetical power station located in central southern England. This case study would be relevant to Task 1 and focus on the impacts arising from emissions of sulphur and nitrogen oxides.
 - Case Study B: a refinery representing a large industrial point source complex. It was agreed that this case study should be based on a representative/hypothetical oil refinery on the south coast of England. This case study would be relevant for ozone and particulate matter (Tasks 1 and 2, respectively).

Protocol for periods in 2003

In this evaluation, the CMAQ model was used in order to quantify reasons for the build up of ozone over South East England during the August 2003 heat wave (Francis *et al.* 2011). The effects of individual meteorological and chemical processes on the temporal evolution of the episode are assessed quantitatively.

Protocol for the footprints

The base case runs for the dynamic evaluation would be the same as used in the earlier operational evaluation. Additional runs were undertaken for the case studies in which the emissions of the facilities are not included:

- Case Study A: a large coal-fired power station source;
- Case Study B: a refinery representing a large industrial point source.

There are no observations of footprints with which to assess the performance of the different models. In this case one of the models was used as the reference for the comparison. The selection of the model (or model configuration) would need to be justified for the particular application. The selection could be based on the performance of the models in the

operational evaluation. It should be understood that the ‘reference’ model is not necessarily correct (or better than the other models). It is simply to allow comparison of the different models.

In addition to the set of performance metrics and graphical presentations, maps of the footprints were produced by subtracting the case study from the base case for the sources of interest. Spatial correlations were also derived.

An additional approach used was based on the simple physics of the processes occurring, as an emulation of a more complex model (Fisher *et al.* 2011). The key diagnostic is taken to be a weighted average concentration given by the average concentration along a typical trajectory, which approximately excludes any dilution arising from dispersion, by multiplying concentration by distance scaled by the concentration value near the source. This is illustrated in Figure 3.2.

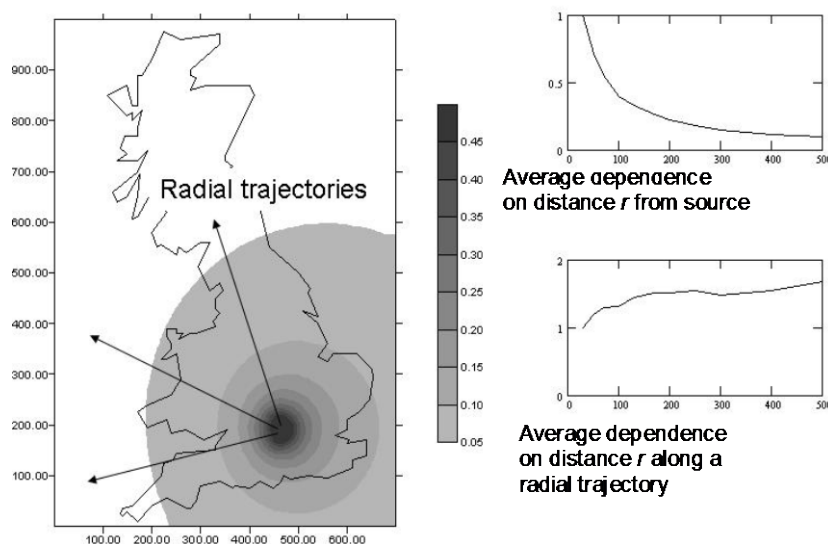


Figure 3.2 Typical example of the annual average PM₁₀ concentration footprint in $\mu\text{g m}^{-3}$ from a major stationary point source such as a power station

The dependence of the PM₁₀ concentration along a trajectory is seen not to decrease rapidly with distance. This can be explained by the gradual formation of secondary aerosol. A key single diagnostic is the distance from the source at which the weighted secondary concentration is at a maximum. This diagnostic summarises the influence of the source on secondary aerosol formation.

The differences between different regional models can be compared by considering the shape of the weighted average concentration dependence on distance and specifically by the distance at which this is a maximum.

3.5 Diagnostic evaluation

As noted by Dennis *et al.* (2010):

an operational evaluation does not provide all the information on the adequacy of models for representing the many interacting physical and chemical processes that lead to the concentrations that are finally modelled.

A diagnostic evaluation is designed to assess the adequacy of the treatment of physical and chemical processes in the model.

One of the key elements of regional air quality models, especially for ground-level ozone, is the chemical mechanism. Different chemical mechanisms are used in the models in the CREMO project. For example, CMAQ uses the carbon-bond mechanism (CBM) (CMAQ v4.5: CBM-IV; CMAQ v4.6/v4.7 used CB05) whereas the OSRM has a lumped explicit formulation (Hayman *et al.* 2010).

There have been many previous intercomparisons of chemical mechanisms. Hough (1988) compared 20 photochemical mechanisms within a trajectory model framework. Derwent (1990) subsequently extended this to 24 chemical mechanisms. There was a major evaluation of chemical mechanisms and global chemical transport models as part of the Intergovernmental Panel on Climate Change (IPCC) Photocomp activity (Olson *et al.* 1997). Kuhn *et al.* (1998) reported an intercomparison of nine chemical mechanisms (including the CBM-IV mechanism).

There have also been a number of studies involving a comparison of a limited set of mechanisms. For example Leucken *et al.* (2008) used the CMAQ model to compare three chemical mechanisms that are widely used in the USA (CBM-IV, CB05 and SPARC-99). The SAPRC-99 mechanism gave higher concentrations than CB05 on average, and both predicted higher ozone concentrations than the CBM-IV mechanism. Yu *et al.* (2010) used the same three mechanisms in the Eta-CMAQ air quality system to simulate the large set of measurements obtained during the 2004 International Consortium for Atmospheric Research on Transport and Transformation (ICARTT) study. Kim *et al.* (2009) reported a comparison of the CB05 and RACM2 chemical mechanisms using the POLAIR3D air quality model. More recently, Chen *et al.* (2010) reported a comparison of five mechanisms (including CB05 and MCM mechanisms) using measurements of the concentrations of hydroxyl (OH) and hydroperoxy (HO₂) from the TexAQS II Radical and Aerosol Measurement Project (TRAMP-2006) field data in 2006. Also using a box model framework, Emmerson and Evans (2009) compared six tropospheric chemistry schemes – including the Common Representative Intermediates (CRI) reduced and CBM-IV – that could be used within composition transport models with the state of the art MCM mechanism.

4 Acceptance criteria

There are no theoretical criteria for model acceptance. The criteria that exist have resulted from expert judgement based on an analysis of actual performance.

In the USA, model performance goals and criteria have been set for ozone (USEPA 1991, Russell and Dennis 2000) and more recently for PM_{2.5} (Boylan and Russell 2006). Boylan and Russell (2006) define performance 'goals' as the level of accuracy that is considered to be close to the best a model can be expected to achieve in that application. Performance 'criteria' are defined as the level of accuracy that is considered to be acceptable for standard modelling applications.

In Europe, the air quality daughter directives specified accuracy criteria for air pollution modelling of the pollutants they cover. In the first daughter directive (covering sulphur dioxide, oxides of nitrogen, carbon monoxide, lead and particulate matter), the accuracy for modelling (and objective estimation) was defined:

as the maximum deviation of the measured and calculated concentration levels, over the period considered by the limit value, without taking into account the timing of the events (EC 1999).

These criteria have generally been retained in the consolidated Air Quality Directive (EC 2008), although the modelling uncertainty is now based on:

the maximum deviation of the measured and calculated concentration levels for 90 % of individual monitoring points, over the period considered, by the limit value (or target value in the case of ozone), without taking into account the timing of the events.

The maximum deviation (also called the maximum Relative Directive Error) should not exceed the modelling objective for the specific pollutant and time period. Further work in this area is in progress through the Forum for Air Quality Modelling in Europe (FAIRMODE) programme.² One of the FAIRMODE activities has been to develop a toolkit to benchmark air quality models.

Derwent *et al.* (2010) recommended two acceptance criteria for the Defra Air Quality Model Evaluation Protocol. These are as follows:

- The fraction of modelled concentrations that lies within ± 50 per cent (that is a factor of two) of the observed value should be greater than 50 per cent.
- The normalised mean bias (*NMB*)³ should be $-0.2 \leq NMB \leq 0.2$ where *NMB* is defined as:

$$NMB = \frac{\sum_{i=1}^N [P_i - O_i]}{\sum_{i=1}^N O_i}$$

²<http://fairmode.ew.eea.europa.eu/models-benchmarking-sg4>

³Note that this is different from mean normalised bias.

where P_i are the calculated values, O_i are the observed values and N is the number of observed-calculated pairs.

Table 4.1 summarises these model acceptance criteria. If all these statistical measures are within the ranges shown, and the graphical performance procedures also are interpreted to yield acceptable results, the model is judged to be performing acceptably.

From preliminary results, models generally comply with the first Defra criterion, so only the second provides a way of discriminating between models. An earlier comparison of simple regional transport models by the Environment Agency for acid deposition (Abbott *et al.* 2001) suggested that regional transport models could be expected to meet the ‘factor of two’ criterion. The 95th percentile of the predicted deposition rates for the simple models available at the time of the study – TRACK, HARM (Hull Acid Rain Model) and FRAME – was within a factor of two of the annual average value and the 5th percentile was within half the annual average value.

One of the advantages of the more complex operational models available today is the ability to test their performance for short-term average concentrations (daily and hourly) and to be able to investigate more fully, complex interactions and feedbacks between processes.

Table 4.1 Specification of model acceptance criteria

Organisation	Species	Model acceptance criteria
USEPA	O ₃	Unpaired highest prediction accuracy: ± 15 –20% Normalised bias: ± 5 –15% Gross error of all pairs >60 parts per billion (ppb): 30–35%
	PM _{2.5}	Mean fractional error (<i>MFE</i>) and the mean fractional bias (<i>MFB</i>) are less than or equal to approximately +50% and ± 30 %, respectively. Additionally the model performance criteria for major components of PM _{2.5} are met when both <i>MFE</i> and <i>MFB</i> are less than or equal to approximately +75% and ± 60 %, respectively.
EU	SO ₂ , NO ₂ , NO _x , CO	Hourly: Relative Directive Error (<i>RDE</i>) 50% Eight-hour averages: <i>RDE</i> 50% Daily averages: <i>RDE</i> 50% Annual averages: <i>RDE</i> 30%
	Benzene	Annual averages: <i>RDE</i> 50%
	PM	Daily averages: not yet defined Annual averages: <i>RDE</i> 50%
	O ₃	Hourly: <i>RDE</i> 50% Eight-hour averages: <i>RDE</i> 50%
UK/Defra	All	The fraction of modelled concentration or metric that lie within ± 50 % of the observed value should be greater than 50%. Normalised mean bias (<i>NMB</i>) should be $-0.2 \leq NMB \leq 0.2$

5 Conclusions and recommendations

Three-dimensional time-dependent numerical models of the atmosphere describe processes at a wide range of spatial and temporal scales. They are used in widely differing applications ranging from research on atmospheric processes to air quality forecasting. For regulatory applications, a model must provide an adequate estimate of concentration response to forcing variables, such as emissions and meteorology, in addition to adequate quantitative estimates of species concentrations.

Model evaluation is a key part of the iterative cycle of model development, testing and confidence building. An important goal of the performance evaluation is to:

- determine a model's degree of acceptability and usefulness for a specified task;
- establish that the model is providing the results for the right reasons.

This report sets out the protocol for the evaluations and model intercomparisons to be undertaken in the CREMO project. It sets out how the evaluation (operational, dynamic and diagnostic) were undertaken and the outputs that were produced.

Consideration has also been given as to whether there are criteria that would determine whether particular models (or model configurations) are acceptable for the specific application. It is concluded that the parameters used in the Defra Model Evaluation Exercise define the minimum acceptable level of model performance:

- The fraction of modelled concentration or metric that lie within ± 50 per cent of the observed value should be greater than 50 per cent.
- The normalised mean bias (*NMB*) should be $-0.2 \leq NMB \leq 0.2$.

The CREMO project has generated some valuable input datasets and model outputs (Fisher *et al.* 2012). It is recommended that these should become a benchmark dataset and made available to the air quality modelling community.

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List of abbreviations

ADMN	Acid Deposition Monitoring Network
ADMS	Atmospheric Dispersion Modelling System
ALPHA	Adapted Low-cost Passive High-Absorption [sampler]
AURN	Automatic Urban and Rural Monitoring Network
BAM	beta attenuation monitor
CBM	carbon-bond mechanism
CEH	Centre for Ecology and Hydrology
CLRTAP	Convention on Long-range Transboundary Air Pollution
CMAQ	Community Multiscale Air Quality
CPC	condensation particle counter
CREMO	Comparison of simple and advanced regional models
CRI	Common Representative Intermediates
Defra	Department for Environment, Food and Rural Affairs
DELTA	DEnuder for Long Term Atmospheric [sampling]
DMS	dimethyl sulphoxide
EC	elemental carbon
EEA	European Environment Agency
EMEP	European Monitoring and Evaluation Programme
EPER	European Pollutant Emission Register
FAC2	factor of two
FAIRMODE	Forum for Air Quality Modelling in Europe
FB	fractional bias
FOEX	Factor of Exceedence
FRAME	Fine Resolution Atmosphere Multi-Pollutant Exchange
GAW	Global Atmospheric Watch [World Meteorological Organization]
HARM	Hull Acid Rain Model
ICARTT	International Consortium for Atmospheric Research on Transport and Transformation
IDA	Inventory Data Analyser
IDOP	integrated downwind ozone production
IPCC	Intergovernmental Panel on Climate Change
IPPC	Integrated Pollution Prevention and Control
IUPAC	International Union of Pure and Applied Chemistry
JEP	Joint Environment Programme
JPL	Jet Propulsion Laboratory

LAQN	London Air Quality Network
LOD	limit of detection
MCIP	Meteorology–Chemistry Interface Processor
MCM	Master Chemical Mechanism
MFE	mean fractional bias
MFE	mean fractional error
NAEI	National Atmospheric Emissions Inventory
NERC	National Environment Research Council
NMB	normalised mean bias
NMSE	normalised mean square error
NMVOC	non-methane volatile organic compound
NO _x	oxides of nitrogen
NRC	National Research Council
OC	organic carbon
OSRM	Ozone Source–Receptor Model
PAN	peroxyacyl nitrates
PM	particulate matter
POCP	photochemical ozone creation potential
ppb	parts per billion
RADM	Regional Acid Deposition Model
RPM	Regional Particulate Model
SEPA	Scottish Environment Protection Agency
SMOKE	Sparse Matrix Operator Kernel Emissions
SNAP	Selected Nomenclature for Air Pollutants
SMPS	scanning mobility particle sizer
TEOM	tapered element oscillating microbalance
TERN	Transport over Europe of Reduced Nitrogen
TRACK	Trajectory model with Atmospheric Chemical Kinetics
TRAMP	TexAQS II Radical and Aerosol Measurement Project
UK PTM	UK Photochemical Trajectory Model
UKEAP	UK Eutrophying and Acidifying Atmospheric Pollutants
UNECE	United Nations Economic Commission for Europe
USEPA	US Environmental Protection Agency
VOC	volatile organic compound
WRF	Weather Research and Forecasting

Appendix 1: Scientific evaluation

Appendix A1.1 contains a template to gather information on the models being used in the CREMO project. Appendix A1.2 provides an overview of the air pollution monitoring networks in the UK relevant to the CREMO project.

A1.1 Template for the model evaluation

Table A1.1 Template for the model evaluation

Model name	
Contact	
Type of model (Eulerian, Lagrangian)	
Model domain(s)	
Applications	
Dry deposition treatment	
Wet deposition treatment	
Chemical scheme	
Meteorology	
Initial/boundary condition	
Emission inventories	
Land cover/land use	
Output chemical species	
Output time resolution	
Platform and runtime(s)	

A1.2 Completed templates for the models used in the model intercomparison

Tables A1.2a to d provide information on the features relevant to the model comparison:

- model domain;
- model physics;
- input data;
- model output.

Table A1.2a Model domain and applications of different models

Model	Type of model	Model domain	Applications
CMAQ	<ul style="list-style-type: none"> • Eulerian • Multi-scale multi-pollutant 	<ul style="list-style-type: none"> • Flexible • One-way nesting 	<ul style="list-style-type: none"> • Urban to regional scale SO₂, NO_x, O₃, PM, deposition • Research and policy model in US
FRAME	<ul style="list-style-type: none"> • Lagrangian • Multi-pollutant 	<ul style="list-style-type: none"> • Covers the British Isles with a fixed grid resolution of 5 km and 33 vertical layers. 	<ul style="list-style-type: none"> • Long-term annual mean deposition of reduced and oxidised nitrogen and sulphur
TRACK-ADMS	<ul style="list-style-type: none"> • Lagrangian for TRACK • Gaussian for ADMS • Multi-pollutant 	<ul style="list-style-type: none"> • UK (20 km resolution) or EMEP (50 km resolution) receptor grids 	<ul style="list-style-type: none"> • Long-term annual mean deposition of reduced and oxidised nitrogen and sulphur • Annual mean concentration for SO₂, NO₂, sulphate and nitrate aerosol, PM₁₀ • Short -term average concentrations for SO₂
OSRM	<ul style="list-style-type: none"> • Lagrangian trajectory • Ozone and oxides of nitrogen 	<ul style="list-style-type: none"> • UK domain • Individual receptors or regular grid (10 km × 10 km). 	<ul style="list-style-type: none"> • Used as ozone policy model in Defra • Large number of O₃ and NO₂ metrics to assess the effects on human health and vegetation
UK PTM	<ul style="list-style-type: none"> • Lagrangian trajectory • Ozone and oxides of nitrogen • PM components 	<ul style="list-style-type: none"> • UK at 10 km × 10 km and EMEP at 50 km × 50 km 	<ul style="list-style-type: none"> • Urban to regional scale O₃ and PM

Table A1.2b Comparison of model physics and chemistry

Models	Dry deposition	Wet deposition	Chemical scheme
CMAQ	<ul style="list-style-type: none"> • Dry deposition scheme based on Pleim-Xiu routine • Hourly deposition velocities calculated for 31 separate species 	<ul style="list-style-type: none"> • Depends on precipitation and considering cloud scavenging effect and aqueous chemistry. 	<ul style="list-style-type: none"> • CB-IV or RADM¹ (both schemes include aqueous and aerosol modules) • CB05 scheme extended to include aqueous and aerosol chemistry • SAPRC99 and mercury chemistry schemes also available
FRAME	<ul style="list-style-type: none"> • Calculated individually to five different land categories • A canopy resistance model for NH₃ • Maps of deposition velocity derived by the CEH 'big leaf' model for SO₂ and NO₂; constant values of deposition velocity for other species. 	<ul style="list-style-type: none"> • A constant drizzle approach using average annual precipitation rates from a climatological map • An enhanced washout rate over hill areas considering the scavenging of cloud droplets by the seeder–feeder effect. • Directionally dependent orographic precipitation 	<ul style="list-style-type: none"> • Similar to EMEP
TRACK-ADMS	<ul style="list-style-type: none"> • Fixed or variable for individual species (land use dependent) 	<ul style="list-style-type: none"> • Constant drizzle approach • Enhanced washout rate over hills (seeder–feeder mechanism) • Directionally dependent orographic precipitation 	<ul style="list-style-type: none"> • Similar to other straight-line acid models used in the UK (such as FRAME and HARM)
OSRM	<ul style="list-style-type: none"> • Conventional resistance approach, diurnal and seasonal dependency 	<ul style="list-style-type: none"> • Not included 	<ul style="list-style-type: none"> • Adapted from STOCHEM • 70 chemical schemes involved in 180 thermal and photochemical reactions
PTM	<ul style="list-style-type: none"> • Determined by dry deposition velocity 	<ul style="list-style-type: none"> • Not included 	<ul style="list-style-type: none"> • MCM

	for the following chemical species: O ₃ , NO ₂ , HNO ₃ , peroxyacyl nitrates (PAN), CO, H ₂ , H ₂ O ₂ , SO ₂ , sulphate and nitrate aerosols, CH ₃ OOH and higher hydroperoxides		<ul style="list-style-type: none">• 4,414 species, 12,871 reactions• 175 emitted man-made VOCs from NAEI + isoprene, α-pinene, β-pinene
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Notes: ¹Regional Acid Deposition Model

Table A1.2c Comparison of model input

Models	Meteorology	Initial/boundary condition	Emissions	Land cover/land use
CMAQ	<ul style="list-style-type: none"> WRF, UM and previously MM5 	<ul style="list-style-type: none"> Monthly average from STOCHEM or observations 	<ul style="list-style-type: none"> GEIA, EMEP, EPER and NAEI. Biogenic emissions calculated based on Guenther <i>et al.</i> (1995) and Sanderson (2002) using CORINE Land Cover data 	<ul style="list-style-type: none"> US Geological Survey (USGS) for dry deposition CORINE¹ for biogenic emissions
FRAME	<ul style="list-style-type: none"> An average annual wind frequency rose giving the appropriate weighting to directional deposition and concentration for calculation of total deposition and average concentration. An average annual wind speed rose used to advect a column of air. The wind statistics were generated from operational radiosonde data from four stations (Dore <i>et al.</i> 2006). UKMO annual average mapped precipitation. 	<ul style="list-style-type: none"> From FRAME-EUROPE (150 km resolution) 	<ul style="list-style-type: none"> SO₂, NO_x and NH₃ (NAEI) with NH₃ emissions disaggregated according to livestock category (Dragosits <i>et al.</i> 1998); No biogenic emissions 	<ul style="list-style-type: none"> Five different land categories (arable, forest, moor-land, grassland and urban) based on CEH land use.
TRACK-ADMS	<ul style="list-style-type: none"> Air parcels arrive at 15° intervals. Contribution of air trajectory is weighted by nearest wind rose (from European Wind Atlas). Average wind speed of 7.5 m s⁻¹ UK precipitation field is obtained from 30-year mean. 	<ul style="list-style-type: none"> Background ozone concentration of 34 ppb OH, CH₃COO₂, NO₃ concentrations obtained from STOCHEM 	<ul style="list-style-type: none"> NAEI and EMEP, estimate of dimethyl sulphide (DMS) emissions from sea 	<ul style="list-style-type: none"> Five different land categories (arable, forest, moor-land, grassland and urban) from RIVM (Netherlands)

Models	Meteorology	Initial/boundary condition	Emissions	Land cover/land use
	<ul style="list-style-type: none"> European precipitation obtained from global long-term average. 			
OSRM	<ul style="list-style-type: none"> Air mass trajectories for each hour are produced for each receptor 	<ul style="list-style-type: none"> Concentrations of O₃, CO, CH₄, C₂H₆, HNO₃ and PAN are initialised for each OSRM trajectory using output from the STOCHEM model. 	<ul style="list-style-type: none"> EMEP and NAEI (eight key sectors); 600 VOC species in NAEI were assigned to 13 modelled species. Biogenic emissions from European forests and agricultural crops based on PELCOM² land cover dataset and the TNO (Netherlands) tree species inventory. 	<ul style="list-style-type: none"> Five generic surface types (urban, grass/heath land, beech trees and crops as winter wheat or potatoes) based on EMEP land cover data
UK PTM	<ul style="list-style-type: none"> Three-dimensional trajectories from Met Office NAME archive, HYSPLIT/NCEP and BADC/Met Office 	<ul style="list-style-type: none"> Observations 	<ul style="list-style-type: none"> EMEP and NAEI VOC speciation for 246 source categories and 663 VOC species Natural emissions from EMEP 	<ul style="list-style-type: none"> Based on Met Office surface exchange scheme

Notes: ¹Coordination of information on the environment (European Commission programme)

²Pan-European Land Use and Land Cover Monitoring

Table A1.2d Comparison of model output

Models	Species	Temporal resolution
CMAQ	More than 36 species including O ₃ , NO ₂ , NO, NO _x , HNO ₃ , SO ₂ , NH ₃ , HONO, PAN, nitrate aerosol, sulphate aerosol, ammonium aerosol, etc.	Hourly
FRAME	NH ₃ , NO, NO ₂ , HNO ₃ , PAN, SO ₂ , H ₂ SO ₄ , as well as NH ₄ ⁺ , NO ₃ ⁻ and SO ₄ ²⁻	Annual average
TRACK-ADMS	PM _{2.5} , PM ₁₀ , NO _x , NO ₂ , HNO ₃ , HONO, PAN, nitrate aerosol, nitrite aerosol, SO ₂ , sulphuric acid, sulphate aerosol, HCl, chloride aerosol, O ₃ , NH ₃ , ammonium aerosol, DMS, H ₂ S, methylsulphonic acid (MSA), NO	Annual
OSRM	Surface concentration of O ₃ and NO ₂ . 70 species.	Hourly
UK PTM	a) O ₃ , PAN and total PANs b) NO, NO ₂ , CO, H ₂ O ₂ , HNO ₃ , NO _z ¹ c) PM sulphate, nitrate, elemental carbon (EC), organic carbon (OC; both natural and man-made) d) Ethylene, toluene, isoprene, formaldehyde e) OH, HO ₂ , RO ₂ f) Ozone budget analysis	15-minute time resolution

Notes: ¹Other nitrogen oxides besides NO_x, such as HNO₃, HONO, organic and particulate nitrates, representing the sum of reaction products

Appendix 2: Measurement networks and methods

This appendix provides an overview of the air pollution monitoring networks in the UK relevant to the CREMO project. The appendix also provides information on the measurement techniques used within these networks. Appendix 3 lists the sites in these different networks together with the species measured in 2003 at each site.

A2.1 Automatic monitoring

A2.1.1 Automatic Urban Rural Network

The Automatic Urban Rural Network (AURN), a Defra funded programme, is the UK's largest automatic monitoring programme. Table A2.1 lists the air pollutants measured and the methods used.

Table A2.1 Pollutants measured by AURN

Pollutant	Method
Oxides of nitrogen (NO _x)	Chemiluminescence
Sulphur dioxide (SO ₂)	UV fluorescence
Ozone (O ₃)	UV absorption
Carbon monoxide (CO)	IR absorption
Particulate matter (as PM ₁₀)	Tapered element oscillating microbalance (TEOM) Beta attenuation monitor (BAM) Gravimetric methods

These methods represent the current state-of-the-art for automated monitoring networks and, with the exception of the automatic PM₁₀ analysers, are the reference methods of measurement defined in the relevant EU air quality directives. There is an extensive programme of quality assurance and quality control of the measurements. The measurements are available from the UK-Air (<http://uk-air.defra.gov.uk/>).

The main objectives of the network are to:

- demonstrate compliance with statutory air quality standards and targets (for example, EU directives);
- provide information to the public about air quality;
- provide information for local air quality review and assessments within the UK Air Quality Strategy;
- identify long-term trends in air pollution concentrations;
- assess the effectiveness of policies to control air pollution.

AURN comprises a variety of site locations across the UK – denoted remote, rural, suburban, urban background, urban centre, kerbside and roadside.

The measurements are reported on an hourly basis from ~120 monitoring sites (August 2008). Of these, 61 were directly funded by Defra and the devolved administrations, while a

further 59 affiliated sites are owned and operated by local authorities; eight of these sites are also in the London Air Quality Network (LAQN). The AURN has expanded dramatically since it was first established in 1992.

A2.1.2 Monitoring by the power generators

As part of the regulatory authorisation, ambient air quality monitoring is undertaken in the vicinity of power stations by the power generating companies. The measurements are reported by the power generators' Joint Environment Programme. The same methods are employed as used in AURN.

A2.2 Deposition monitoring

The monitoring of deposition was previously undertaken in a number of separate networks supported by Defra (Acid Deposition Monitoring Network, HNO₃ Denuder Network and Ammonia Monitoring Network). In 2009, these networks were rationalised to form the UK Eutrophying and Acidifying Atmospheric Pollutants (UKEAP) monitoring programme. Additional measurements are also made as part of the National Environment Research Council (NERC) Environmental Change Network. Some of the sites are common to the NERC and Defra networks.

The measurements made in the Defra supported networks are described in the following sections.

A2.2.1 Precipitation composition

In 2003, fortnightly precipitation samples were collected at 38 sites using bulk collectors based on the design of Hall (1986). Daily measurements of precipitation composition were also made at Eskdalemuir, again using a bulk collector. Stone and Tily (1992) provided an assessment of the collection efficiency of the bulk collector. For the two-year period 1986 to 1987, the bulk collector was found to have collection efficiencies, which ranged from 77% to 99% compared with the five-inch meteorological rain gauge.

The precipitation samples were analysed using ion chromatography and the concentrations of H⁺, Na⁺, K⁺, Mg²⁺, Ca²⁺, NH₄⁺, SO₄²⁻, NO₃⁻, Cl⁻ present were determined. Concentrations of phosphate (PO₄³⁻) were also determined and these were used as an indicator of possible sample contamination. Concentrations of non-sea salt sulphate were derived by difference from the total sulphate concentration, the concentration of Na⁺ and the composition of sea water being used to calculate the concentration of sea salt sulphate.

The sampling frequency was changed from weekly to fortnightly in 2001. An intercomparison exercise was undertaken between 2001 and 2005 using three sites: Eskdalemuir, Lough Navar and Thorganby (Hayman *et al.* 2004, 2005). The results from the first three years of the intercomparison indicated that there was good agreement between the parameters collected for the different sampling durations (Hayman *et al.* 2005).

A2.2.2 Sulphur dioxide and particulate sulphate

Measurements of sulphur dioxide were made at about 40 rural sites between 1986 and 2006. Until 2001, daily measurements of sulphur dioxide and particulate sulphate were made at eight sites using a single sampler – the eight-port hydrogen peroxide bubbler instrument (AGL, Hitchin). Weekly measurements were also made at a further 32 sites in the Rural SO₂ Monitoring network. Air was drawn through a filter (to remove particulate

sulphate) and passed through a bubbler containing hydrogen peroxide. Sulphur dioxide was oxidised to sulphate, which was then determined by ion chromatography. At the other sites weekly measurements were made with the bubbler instrument.

With the decline in emissions of sulphur dioxide in the UK, the concentrations of sulphur dioxide measured at some of the sites, especially those in remote areas, were at or below the limit of detection (LOD) of the bubbler method. Following a method intercomparison exercise (Hasler et al. 2000), the filter pack sampler was introduced in 2001.

The filter pack sampler consists of two filters in series enclosed in an airtight holder. Air is drawn through the filter pack and sulphate aerosol particles are removed on the first filter. Sulphur dioxide is absorbed by the second filter, which has been previously washed with potassium carbonate and then impregnated with a glycerol/potassium hydroxide solution. The sulphur dioxide is quantitatively converted to solid potassium sulphite by reaction with the potassium hydroxide and oxidising species in the air convert the sulphite to sulphate during sampling. The sulphate on the exposed impregnated filter is extracted using water. The sulphate concentration in the solution is determined using ion chromatography and this is converted into a gas-phase concentration of sulphur dioxide. The sampling frequency was initially fortnightly and then four-weekly sampling from the beginning of 2004.

The filter pack sampling programme was stopped at the end of 2005. Since then, SO₂ measurements have been made as part of an expanded HNO₃ denuder network (see Section A2.2.4). Half of the 30 sites in the expanded were previously part of the Rural SO₂ Monitoring Network.

The eight-port sampler continued to be used to determine concentrations of particulate sulphate on a daily basis at five sites. Particulate sulphate was collected by drawing air through a Whatman 40 filter and the sulphate concentrations were determined by ion chromatography. This sampling programme was terminated in April 2009.

A2.2.3 Nitrogen dioxide

Nitrogen dioxide concentrations were and are still measured at deposition sites using passive diffusion tubes. The gas species of interest diffuses up the tube and is collected on an efficient absorbent medium at the closed end. The amount of gas absorbed is then analysed. The tube components were manufactured to a 0.1 mm tolerance, providing a known diffusion path length and hence a constant resistance to uptake. The ambient concentration of the gas can then be calculated from the diffusion path length, amount absorbed (determined analytically), exposure time and diffusion coefficient of the gas.

Diffusion tubes have been used to measure nitrogen dioxide concentrations. Tubes are mounted on the upright of the rain collector stand and are exposed for 12 four or five-week periods throughout each year. This was set to four-week periods in 2005 to coordinate sample changeovers with the fortnightly rain collections.

Further changes have been made since 2003. There has been a reduction in the number of sites following the introduction of automatic NO_x analysers at rural locations and the introduction of best practice in diffusion tube measurements (especially the use of triplicate tubes at three sites where there are also automatic NO_x analysers and bias corrections).

A2.2.4 Delta denuder technique

In 2003, nitric acid and related species were monitored on a monthly basis at 12 locations using the CEH DELTA (DEnuder for Long Term Atmospheric sampling) system in an integrated fashion with the UK Ammonia Monitoring Network (see Section A2.3). The aim of these measurements is to:

- explore spatial patterns;
- compare results with dispersion models and seasonality;
- contribute to national nitrogen deposition estimates.

The sampling train used in the denuder system is shown Figure A2.1. HNO_3 , SO_2 and HCl are removed by the first set of K_2CO_3 /glycerol coated denuders, and a second set of citric acid coated denuders removes NH_3 . Two sets of filter packs at the end of the sampling train remove the aerosol components (NO_3^- , SO_4^{2-} , Cl^- and NH_4^+).

Samples are stored in a cold room at 4°C until analysis. For the denuders, 5 ml of 0.05 per cent H_2O_2 is added to both the first and second denuders, while the initial uncoated short length of Teflon inlet is not extracted. Filters from the filter packs are also extracted in 0.05 per cent H_2O_2 . Extracted aqueous samples from the denuders and the filter packs are analysed for NO_3^- , SO_4^{2-} and Cl^- and filter sample extracts are analysed for NO_3^- , SO_4^{2-} , Cl^- , Na^+ , Mg^{2+} and Ca^{2+} .

In 2006, the network was expanded to 30 sites.

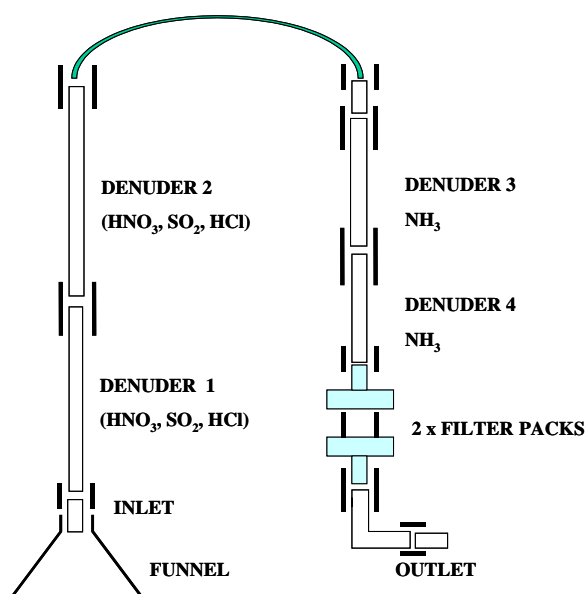


Figure A2.1 Sampling train for monthly air measurements

A2.2.5 Ammonia monitoring

There are currently 95 sites in the National Ammonia Monitoring Network. The high spatial variability of ammonia concentrations demonstrates that this large number of sites is necessary. At 59 of these sites, an active diffusion denuder methodology using the CEH DELTA system (where power is available) is used to provide the main spatial and temporal patterns of NH_3 across the UK (see Section A2.2.4). Aerosol NH_4^+ , a secondary product, is spatially more even and is monitored at a subset of the DELTA sites.

The denuder network is complemented by a secondary network of ALPHA (Adapted Low-cost Passive High-Absorption) samplers at a further 49 sites to assess regional and local scale variability in air NH_3 concentrations in source regions. The ALPHA sampler was designed and developed specifically for monitoring ambient concentrations of NH_3 , with a detection limit of around $0.02 \mu\text{g NH}_3 \text{ m}^{-3}$ for monthly monitoring. To provide an ongoing

validation of the ALPHA sampler, the method is calibrated against the DELTA method at 12 sites within the network.

A2.3 Monitoring of particulate matter

Measurements are made of:

- particle number concentrations;
- particle size distributions;
- composition of particulate matter in different sizes (PM_{2.5} and PM₁₀).

A brief summary of the operation of each instrument is given below.

A2.3.1 Particle counting and sizing analysers

These instruments operate on the principle of passing the sample through clean air supersaturated with butanol, causing a butanol droplet to form around each particle so that they can be counted optically. In a condensation particle counter (CPC), the total number concentrations of particles in the size range ~7nm to several microns are determined in this way, either by individual number counting (at low concentrations) or using an optical integrating method (at high concentrations). In the case of a scanning mobility particle sizer (SMPS), the sample entering the CPC has passed through air ionised by a radioactive device (based on Krypton-85) which gives an electric charge to a known fraction of the particles, and then through a controlled electrical potential that separates the charged particles according to their electrical mobility.

A2.3.2 Automated nitrate and carbon analysers

Both systems operate on broadly similar principles. For the nitrate analyser, the particulate content of the air is sampled onto a flash strip via an internal cyclone inlet. For the carbon analyser, the particulate content of the air is sampled through a size selective inlet and then collected by an impactor. In the case of the nitrate analysers, the system flash heats the particulate matter and the quantity of NO_x produced is analysed, and in the case of the carbon analysers, CO₂ is produced. In the latter case the combustion is initially performed at a temperature of 320–370°C to determine the organic carbon content and subsequently at a temperature of 650–700°C to determine the elemental or 'soot' carbon content.

Since May 2007, elemental carbon (EC) and organic carbon (OC) concentrations in ambient air have been determined from filters. Between May 2007 and October 2007, the determination was made from quartz fibre filters provided by Bureau Veritas. The filter type was switched in the 'anion' Partisol samplers from Emfab (PTFE-coated glass fibre) to ultrapure quartz to allow for the analysis of EC/OC. A punch is taken from each filter and analysed for elemental and organic carbon in a procedure in which the measurand is method-defined. It involves heating the sample to remove the carbon from the filter and conversion to methane, followed by detection by flame ionisation. In a helium atmosphere, the sample is gradually heated to 700°C to remove all organic carbon on the filter. During this first phase, there are usually some organic compounds that are pyrolytically converted to elemental carbon. (Measuring the transmission of a laser beam through the filter continuously monitors this pyrolytic conversion and allows a correction to be made for it.) Elemental carbon is detected in the same way after heating to 870°C in the presence of oxygen and helium.

A2.3.3 Inorganic anions (sulphate, nitrate and chloride)

Daily measurements of the inorganic components of PM₁₀ (sulphate, nitrate and chloride) were made using a Thermo Partisol 2025 sequential air sampler. Until October 2007, the PM₁₀ samples were collected on glass fibre filters (Emfab, PTFE-bound glass fibre). From October 2007, ultrapure quartz filters have been used to allow for the analysis of EC/OC in addition to the inorganic components.

The Partisol sampler provides uninterrupted sampling of ambient air and automatic exchange of filters for up to 16 days. The instrument used an airflow of 16.7 litres per minute through a PM₁₀ inlet and the filter temperature was maintained to within $\pm 5^{\circ}\text{C}$ of ambient temperature. The exposed filters were stored in small polypropylene filter bags and kept in a cold room until analysis to prevent further loss of volatile components. Extracts from the filters were dissolved in an eluent of 3.5mM sodium carbonate and 1mM sodium hydrogen carbonate, and analysed in the laboratory by ion chromatography for sulphate, nitrate and chloride content. Ambient concentrations were derived from the mass measured on the filter and the airflow during the sampling period.

Appendix 3: Sites and measurements used in the model evaluation

Network group	Site name	Longitude	Latitude	Network																						
				AURN					JEP				Particle			UKEAP										
				O ₃ (hourly)	NO/NO ₂ /NOx(hourly)	SO ₂ (hourly)	CO (hourly)	PM ₁₀ (hourly)	PM _{2.5} (hourly)	O ₃ (hourly)	NO/NO ₂ /NOx (hourly)	SO ₂ (hourly)	PM ₁₀ (hourly)	Met (hourly)	Particle Number (hourly)	SMPS (hourly)	Partisol Filter (daily)	NO ₃ (hourly)	EC/OC (hourly)	Precipitation (daily, bulk)	Precipitation (fortnightly,	NO ₂ (monthly)	SO ₂ (fortnightly)	SO ₄ (daily)	HNO ₃ denuder (monthly)	NH ₃ (monthly)
UKEAP(NH ₃)	5 Acres	-5.0977	50.2954																							X
AURN (Urban Background)	Aberdeen	-2.0942	57.1566		X	X	X	X																		
UKEAP(Precip., NO ₂)	Achanarras	-3.4558	58.4753																		X	X				
UKEAP(NH ₃)	Alice Holt	-0.8436	51.1341																							X
UKEAP(Precip., NO ₂ , NH ₃)	Allt a' Mharcaidh	-3.8567	57.1242																		X	X				X
UKEAP(SO ₂)	Appleacre	0.0000	0.0000																				X			
AURN (Rural)	Aston Hill	-3.0342	52.5042	X																						
UKEAP(NH ₃)	Aston Rowant.	-0.9485	51.6747																							X
UKEAP(NH ₃ , SO ₂)	Auchencorth Moss	-3.2426	55.7928																				C			X
UKEAP(NH ₃)	Auchincruive	-4.5652	55.4775																							X
UKEAP(Precip., NO ₂)	Balquhidder	-4.3939	56.3547																		X	X				
UKEAP(Precip., NO ₂)	Bannisdale	-2.7478	54.4317																		X	X				
UKEAP(Precip., NO ₂ , SO ₂ , NH ₃)	Barcombe Mills	0.0444	50.9150																		X	X	X	X	X	X
AURN (Urban Background)	Barnsley 12	-1.4837	53.5540				X																			
AURN (Urban Background)	Barnsley Gawber	-1.5108	53.5631	X	X	X	X																			
JEP (South Trent Valley)	Bass Burton Brewery	-1.6380	52.8058							X	X															
UKEAP(Precip.)	Beaghs Burn	-0.1031	55.0833																		X					
UKEAP(NH ₃)	Bedlingfield	1.1852	52.2703																							X
AURN (Urban Centre)	Belfast Centre	-5.9279	54.5996	X	X	X	X	X							X		X	X	X							
AURN (Urban Background)	Belfast East	-5.9013	54.5959				X																			
UKEAP(SO ₂)	Benniguniea	-	-																				X			
JEP (Midlands)	Bentley Hall Farm	-1.8755	52.7676							X	X															
UKEAP(SO ₂)	Bentra	-	-																				X			
JEP (Thames Estuary)	Bexleyheath	0.1328	51.4501							X	X															
UKEAP(NH ₃)	Bickerton Hill	-2.7493	53.0689																							X
AURN (Urban Industrial)	Billingham	-1.2739	54.6063		X																					

Network group	Site name	Longitude	Latitude	Network																						
				AURN						JEP				Met (hourly)	Particle				UKEAP							
				O ₃ (hourly)	NO/NO ₂ /NOx(hourly)	SO ₂ (hourly)	CO (hourly)	PM ₁₀ (hourly)	PM _{2.5} (hourly)	O ₃ (hourly)	NO/NO ₂ /NOx (hourly)	SO ₂ (hourly)	PM ₁₀ (hourly)			Particle Number (hourly)	SMPS (hourly)	Partisol Filter (daily)	NO ₃ (hourly)	EC/OC (hourly)	Precipitation (daily, bulk)	Precipitation (fortnightly,	NO ₂ (monthly)	SO ₂ (fortnightly)	SO ₄ (daily)	HNO ₃ denuder (monthly)
AURN (Urban Centre)	Birmingham Centre	-1.9087	52.4800	X	X	X	X	X							X											
AURN (Urban Background)	Bolton	-2.4394	53.5732	X	X	X	X	X																		
AURN (Suburban), Precip.)	Bottesford	-0.8143	52.9308	X																	X	X				
JEP (South Trent Valley)	Bottesford	-0.8158	52.9299							X	X	X	X	X												
AURN (Urban Background)	Bournemouth	-1.8271	50.7391	X	X	X		X																		
JEP (Aberthaw)	Boverton Mill Farm	-3.4488	51.3949								X	X														
AURN (Urban Centre)	Bradford Centre	-1.7495	53.7931	X	X	X	X	X																		
UKEAP(SO ₂)	Brockhill 1	0.0000	0.0000																				C			
UKEAP(NH ₃)	Brompton	-1.4010	54.3831																							X
UKEAP(NH ₃)	Brown Moss NR 2	-2.6504	52.9463																							X
UKEAP(NH ₃)	Bure Marshes	1.4542	52.6918																							X
AURN (Rural), UKEAP(NH ₃ , SO ₂)	Bush Estate	-3.2063	55.8624	X																			X		X	X
UKEAP(SO ₂)	Bylchau	-	-																				X			
UKEAP(SO ₂)	Caenby 1	-	-																				X			
UKEAP(SO ₂)	Cam Forest	-	-																				C			
UKEAP(SO ₂)	Camborne 1	-	-																				X			
UKEAP(SO ₂)	Camphill 1	-	-																				X			
AURN (Urban Background)	Canterbury	1.0983	51.2738		X			X																		
AURN (Urban Centre)	Cardiff Centre	-3.1765	51.4815	X	X	X	X	X																		
UKEAP(SO ₂)	Cardington 2	0.0000	0.0000																				C			
UKEAP(NH ₃)	Cardoun Burn	-4.2715	54.9655																							X
UKEAP(NH ₃)	Carlisle	-2.8295	54.8904																							X
JEP (Aire Valley)	Carr Lane, Drax	-0.9827	53.7386								X															X
UKEAP(NH ₃)	Carradale	-5.4944	55.5840																							X
UKEAP(NH ₃)	Castle Cary	-2.5583	51.0846																							X
UKEAP(SO ₂)	Church Fenton	-	-																				X			
UKEAP(NH ₃)	Coalburn	-2.4811	55.0972																							X
UKEAP(NH ₃)	Coleraine	-6.6050	55.0405																							X
UKEAP(Precip.)	Compton	-1.2619	51.5197																		X	X				
UKEAP(SO ₂)	Corpach 1	0.0000	0.0000																				X			
AURN (Urban Background)	Coventry Memorial Park	-1.5194	52.3927	X	X	X	X	X																		
UKEAP(Precip.)	Cow Green Reservoir	-2.2836	54.6628																		X	X				
UKEAP(Precip., SO ₂)	Crai Reservoir	-3.6194	51.8903																		X		X			
UKEAP(SO ₂)	Cresselly 1	-	-																				X			
JEP (North Trent Valley)	Cromwell	-0.8082	53.1509							X	X	X		X												
AURN (Urban Background)	Cwmbran	-3.0060	51.6530		X	X	X	X																		

Network group	Site name	Longitude	Latitude	Network																						
				AURN						JEP					Particle				UKEAP							
				O ₃ (hourly)	NO/NO ₂ /NOx(hourly)	SO ₂ (hourly)	CO (hourly)	PM ₁₀ (hourly)	PM _{2.5} (hourly)	O ₃ (hourly)	NO/NO ₂ /NOx (hourly)	SO ₂ (hourly)	PM ₁₀ (hourly)	Met (hourly)	Particle Number (hourly)	SMPS (hourly)	Partisol Filter (daily)	NO ₃ (hourly)	EC/OC (hourly)	Precipitation (daily, bulk)	Precipitation (fortnightly, NO ₂ (monthly)	SO ₂ (fortnightly)	SO ₄ (daily)	HNO ₃ denuder (monthly)	NH ₃ (monthly)	
UKEAP(NH ₃ , SO ₂)	Cwmystwyth	-	-																				X		X	X
UKEAP(NH ₃)	Dennington	1.3349	52.2527																							X
AURN (Urban Background)	Derry	-7.3287	55.0004	X	X	X	X	X																		
JEP (Didcot)	Didcot North	-1.2556	51.6478							X	X	X		X												
JEP (Didcot)	Didcot South, Winaway Kennels	-1.3013	51.5924							X	X	X														
JEP (Aire Valley)	Downes Ground Farm	-0.9347	53.7158								X	X	X													
UKEAP(NH ₃ , SO ₂)	Drayton	-1.7630	52.1935																							
UKEAP(Precip.)	Driby	0.0775	53.2483																		X	X				
UKEAP(NH ₃)	Dunwich Heath	1.6194	52.2542																							X
UKEAP(NH ₃)	Easingwold	-1.1741	54.1004																							X
JEP (Thames Estuary)	East Tilbury, Bowaters Farm	0.4102	51.4690							X	X															X
UKEAP(NH ₃)	Ellon Ythan	-2.0914	57.3642																							X
AURN(Rural)	Eskdalemuir	-3.2069	55.3151	X																	X	X	X	X	X	X
UKEAP(SO ₂)	Etton 1	-	-																							
UKEAP(SO ₂)	Fairseat	-	-																							
UKEAP(NH ₃)	Fenn's Moss 1	-2.7587	52.9232																							X
UKEAP(Precip., NO ₂)	Flatford Mill	1.0233	51.9589																		X	X				
JEP (Aberthaw)	Font-y-Gary	-3.3623	51.3860							X	X	X														
UKEAP(SO ₂)	Formoyle	-	-																							
UKEAP(SO ₂)	Forsinain/Forsinard	-	-																							
UKEAP(SO ₂)	Fort Augustus 2	-	-																							
UKEAP(NH ₃)	Fressingfield	1.3190	52.3341																							X
JEP (North Trent Valley)	Gainsborough Cemetery	-0.7695	53.4058							X	X															
UKEAP(SO ₂)	Garrary	-	-																							
JEP (Thames Estuary)	Gillingham	0.5630	51.3947							X	X			X												
AURN (Urban Background)	Glasgow Centre	-4.2559	55.8575	X	X	X	X	X								X										
AURN (Urban Background)	Glasgow City Chambers	-4.2464	55.8604																							
AURN (Suburban)	Glazebury	-2.4729	53.4598	X																						
UKEAP(Precip., NO ₂)	Glen Dye	-2.5889	56.9675																		X	X	X	C		
UKEAP(NH ₃)	Glensaugh	-2.5518	56.9094																							X
UKEAP(NH ₃)	Glenshee Hotel	-3.4563	56.8122																							X
UKEAP(Precip., NO ₂)	Goonhilly	-5.1811	50.0483																		X	X				
AURN (Urban Industrial)	Grangemouth	-3.7049	56.0102		X	X		X																		
AURN (Remote)	Great Dun Fell	-2.4513	54.6840	X																						

Network group	Site name	Longitude	Latitude	Network																						
				AURN					JEP					Particle					UKEAP							
				O ₃ (hourly)	NO/NO ₂ /NOx (hourly)	SO ₂ (hourly)	CO (hourly)	PM ₁₀ (hourly)	PM _{2.5} (hourly)	O ₃ (hourly)	NO/NO ₂ /NOx (hourly)	SO ₂ (hourly)	PM ₁₀ (hourly)	Met (hourly)	Particle Number (hourly)	SMPS (hourly)	Partisol Filter (daily)	NO ₃ (hourly)	EC/OC (hourly)	Precipitation (daily, bulk)	Precipitation (fortnightly, monthly)	NO ₂ (monthly)	SO ₂ (fortnightly)	SO ₄ (daily)	HNO ₃ denuder (monthly)	NH ₃ (monthly)
JEP (North Trent Valley)	Grove Reservoir	-0.8885	53.3153							X	X	X		X												X
UKEAP(NH ₃)	Gulabin Lodge	-3.4580	56.8140																							X
UKEAP(NH ₃)	Halladale	-3.8797	58.4141																							X
AURN (Rural)	Harwell	-1.3261	51.5709	X	X	X		X						X	C	X	X	X	X							
UKEAP(SO ₂)	Hebden Bridge 2	-	-																				X			
JEP (Aire Valley)	Hemingbrough Landing	-0.9867	53.7593								X	X														
AURN(Rural)	High Muffles	-0.8096	54.3348	X																		X	X	X	X	X
UKEAP(Precip., NO ₂ , NH ₃ , SO ₂)	Hillsborough	-6.0607	54.4670																							X
UKEAP(Precip., NO ₂)	Hillsborough Forest	-6.0842	54.4525																			X	X			
UKEAP(NH ₃)	Holme Lacy	-2.6500	52.0175																							X
AURN (Urban Centre)	Hull Freetown	-0.3409	53.7486	X	X	X	X	X																		
UKEAP(SO ₂)	Husborne Crawley 1	-	-																				X			
UKEAP(NH ₃)	Inverpollly	-5.0708	58.0315																							X
UKEAP(Precip., NO ₂)	Jenny Hurn	-0.7703	53.4775																		C	C				
AURN (Rural)	Ladybower	-1.7518	53.4030	X	X	X																				
UKEAP(NH ₃)	Lagganlia	-3.8891	57.1102																							X
UKEAP(NH ₃)	Lakes	-3.0198	54.3380																							X
AURN (Urban Background)	Leamington Spa	-1.5338	52.2885	X	X	X	X	X																		
AURN (Urban Centre)	Leeds Centre	-1.5459	53.8041	X	X	X	X	X																		
AURN (Urban Centre)	Leicester Centre	-1.1327	52.6315	X	X	X	X	X																		
UKEAP(NH ₃)	Little Budworth	-2.6226	53.1874																							X
UKEAP(SO ₂)	Little Horkesley 1	-	-																				X			
UKEAP(NH ₃)	Llydaw	-3.9492	53.0957																							X
UKEAP(Precip., NO ₂ , NH ₃)	Llyn Brianne	-3.7296	52.1208																		X	X				X
UKEAP(Precip., NO ₂)	Llyn Llgi	-4.0394	53.0300																		X					
UKEAP(Precip., NO ₂)	Llyn Llydaw	-4.0283	53.0764																		X	X				
UKEAP(NH ₃)	Llynclys Common	-3.0786	52.8056																							X
UKEAP(NH ₃)	Loch Awe	-5.2837	56.2525																							X
UKEAP(Precip.)	Loch Chon	-4.5358	56.2478																		X					
UKEAP(Precip., NO ₂)	Loch Dee	-4.3997	55.0719																		X	X				
UKEAP(SO ₂)	Loch Leven 2	-	-																				X			
UKEAP(Precip.)	Lochnagar	-3.2308	56.9581																		X					
AURN (Suburban)	London Bexley	0.1854	51.4661	X	X	X	X	X																		
AURN (Urban Centre)	London Bloomsbury	-0.1262	51.5219	X	X	X	X	X	X						X	X										
AURN (Urban Background)	London Brent	-0.2749	51.5898	X	X	X	X	X																		

Network group	Site name	Longitude	Latitude	Network																						
				AURN						JEP					Particle				UKEAP							
				O ₃ (hourly)	NO/NO ₂ /NOx(hourly)	SO ₂ (hourly)	CO (hourly)	PM ₁₀ (hourly)	PM _{2.5} (hourly)	O ₃ (hourly)	NO/NO ₂ /NOx (hourly)	SO ₂ (hourly)	PM ₁₀ (hourly)	Met (hourly)	Particle Number (hourly)	SMPS (hourly)	Partisol Filter (daily)	NO ₃ (hourly)	EC/OC (hourly)	Precipitation (daily, bulk)	Precipitation (fortnightly,	NO ₂ (monthly)	SO ₂ (fortnightly)	SO ₄ (daily)	HNO ₃ denuder (monthly)	NH ₃ (monthly)
AURN (Suburban)	London Eltham	0.0708	51.4526	X	X	X		X																		
AURN (Urban Centre)	London Hackney	-0.0567	51.5588	X	X		X																			
AURN (Urban Centre)	London Haringey	-0.1262	51.5860	X																						
AURN (Suburban)	London Hillingdon	-0.4614	51.4962	X	X	X	X	X																		
AURN (Urban Centre)	London Lewisham	-0.0202	51.4454	X	X	X																				
AURN (Urban Background)	London N. Kensington	-0.2136	51.5209	X	X	X	X	X	X						X	C	X		X							
AURN (Urban Centre)	London Southwark	-0.0965	51.4905	X	X	X	X																			
AURN (Urban Background)	London Teddington	-0.3403	51.4208	X	X	X																				
AURN (Urban Centre)	London Wandsworth	-0.1910	51.4571	X	X																					
AURN (Urban Background)	London Westminster	-0.1316	51.4941	X	X	X	X																			
AURN(Rural)	Lough Navar	-7.8758	54.4430																			X	X	X	X	X
UKEAP(Precip., NO ₂ , NH ₃ , SO ₂)	Lullington Heath	0.1809	50.7935	X	X	X																				X
AURN (Rural), UKEAP(NH ₃)	Lyulphs Tower	-2.9236	54.5734																							X
UKEAP(NH ₃)	Manchester Piccadilly	-2.2381	53.4812	X	X	X	X	X							X											
AURN (Urban Background)	Manchester South	-2.2434	53.3688	X	X	X																				
AURN (Urban Background)	Manchester Town Hall	-2.2441	53.4785		X		X																			
UKEAP(SO ₂)	Marshfield 1	-	-																							
JEP (North Trent Valley)	Marton	-0.7343	53.3268							X	X	X		X												
UKEAP(NH ₃)	Marton	-0.7326	53.3270																							X
UKEAP(NH ₃)	Mere Sands Wood	-2.8364	53.6347																							X
AURN (Urban Industrial)	Middlesbrough	-1.2204	54.5673	X	X	X	X	X																		
UKEAP(NH ₃)	Moor House	-2.3864	54.6949																							X
UKEAP(NH ₃)	Myerscough	-2.7632	53.8527																							X
AURN (Remote)	Narberth	-4.6892	51.7821	X	X	X		X																		
AURN (Urban Centre)	Newcastle Centre	-1.6109	54.9781	X	X	X	X	X																		
JEP (Aire Valley)	North Featherstone	-1.3547	53.6990								X	X														
UKEAP(NH ₃)	North Wyke	-3.9019	50.7682																							X
UKEAP(NH ₃)	Northallerton	-1.4463	54.3311																							X
AURN (Urban Background)	Northampton	-0.8861	52.2734	X	X	X		X																		
JEP (Thames Estuary)	Northfleet	0.3385	51.4479							X	X															
AURN (Urban Centre)	Norwich Centre	1.2954	52.6319	X	X	X	X	X																		
AURN (Urban Centre)	Nottingham Centre	-1.1470	52.9552	X	X	X	X	X																		
UKEAP(NH ₃)	Oldmeldrum	-2.2791	57.3361																							X
UKEAP(NH ₃)	Orielton	-4.9581	51.6538																							X
UKEAP(NH ₃)	Penallt	-2.6915	51.7817																							X

Network group	Site name	Longitude	Latitude	Network																						
				AURN						JEP					Particle				UKEAP							
				O ₃ (hourly)	NO/NO ₂ /NO _x (hourly)	SO ₂ (hourly)	CO (hourly)	PM ₁₀ (hourly)	PM _{2.5} (hourly)	O ₃ (hourly)	NO/NO ₂ /NO _x (hourly)	SO ₂ (hourly)	PM ₁₀ (hourly)	Met (hourly)	Particle Number (hourly)	SMPS (hourly)	Partisol Filter (daily)	NO ₃ (hourly)	EC/OC (hourly)	Precipitation (daily, bulk)	Precipitation (fortnightly, monthly)	NO ₂ (monthly)	SO ₂ (fortnightly)	SO ₄ (daily)	HNO ₃ denuder (monthly)	NH ₃ (monthly)
UKEAP(SO ₂)	Pitlochry	-	-																							
AURN (Urban Centre)	Plymouth Centre	-4.1431	50.3715	X	X	X	X	X																		
UKEAP(NH ₃)	Pointon	-0.3241	52.8670																							X
UKEAP(NH ₃)	Pointon 3	-0.3241	52.8670																							X
UKEAP(Precip., NO ₂)	Polloch	-5.6128	56.7508																		X	X				
AURN (Urban Industrial)	Port Talbot	-3.7621	51.5794	X	X	X		X							X											
UKEAP(NH ₃)	Porton Down	-1.6384	51.1267																							X
AURN (Urban Background)	Portsmouth	-1.0685	50.8282		X	X	X	X	X																	
AURN (Urban Background)	Preston	-2.6811	53.7653	X	X	X	X	X	X																	
UKEAP(Precip., NO ₂)	Preston Montford	-2.8381	52.7231																		X	X	X			
UKEAP(Precip., NO ₂)	Pumlumon	-3.7322	52.4536																		X	X				
UKEAP(NH ₃)	Pwllpeiran	-3.7661	52.3783																							X
UKEAP(NH ₃)	Rannoch	-4.2788	56.6507																							X
UKEAP(SO ₂)	Ratcliffe 13	-	-																					C		
AURN (Suburban)	Redcar	-1.0725	54.6130	X	X	X	X	X																		
UKEAP(Precip., NO ₂)	Redesdale	-2.2628	55.2497																		X	X	X			
UKEAP(NH ₃)	Redgrave + Lopham	1.0121	52.3765																							X
UKEAP(Precip.)	River Etherow	-2.3586	53.8108																		X					
JEP (Thames Estuary)	Rochester	0.6340	51.4552							X	X															
AURN (Rural)	Rochester Stoke	0.6340	51.4551	X	X	X		X	X					X												
UKEAP(SO ₂)	Rockbourne 1	-	-																				X			
JEP (Didcot)	Rosehurst Farm	-1.2082	51.6295							X	X	X	X	X												
UKEAP(SO ₂)	Rosemaund	-	-																				X			
UKEAP(NH ₃)	Rothamstead	-0.3711	51.8030																						X	X
AURN (Urban Centre)	Rotherham Centre	-1.3528	53.4320	X	X	X																				
UKEAP(NH ₃)	Ruabon	-3.1558	53.0315																							X
JEP (South Trent Valley)	Ruddington Fields	-1.1633	52.8834								X	X		X												
UKEAP(NH ₃)	Rum	-6.2701	57.0111																							X
JEP (Fiddler's Ferry)	Runcom Town Hall	-2.7227	53.3341							X	X															
JEP (Fiddler's Ferry)	Sacred Heart School	-2.6148	53.3891							X	X		X													
AURN (Urban Industrial)	Salford Eccles	-2.3345	53.4845	X	X	X	X	X																		
AURN (Urban Background)	Sandwell West Bromwich	-1.9970	52.5214	X	X	X	X																			
UKEAP(NH ₃)	Savarnake	-1.9206	51.5975																							X
UKEAP(Precip.)	Scoat Tarn	-3.5028	54.8028																							
AURN (Urban Centre)	Sheffield Centre	-1.4738	53.3769	X	X	X	X	X													X					
AURN (Urban Industrial)	Sheffield Tinsley	-1.3967	53.4107		X		X																			

Network group	Site name	Longitude	Latitude	Network																						
				AURN						JEP					Particle			UKEAP								
				O ₃ (hourly)	NO/NO ₂ /NOx(hourly)	SO ₂ (hourly)	CO (hourly)	PM ₁₀ (hourly)	PM _{2.5} (hourly)	O ₃ (hourly)	NO/NO ₂ /NOx (hourly)	SO ₂ (hourly)	PM ₁₀ (hourly)	Met (hourly)	Particle Number (hourly)	SMPS (hourly)	Partisol Filter (daily)	NO ₃ (hourly)	EC/OC (hourly)	Precipitation (daily, bulk)	Precipitation (fortnightly,	NO ₂ (monthly)	SO ₂ (fortnightly)	SO ₄ (daily)	HNO ₃ denuder (monthly)	NH ₃ (monthly)
UKEAP(NH ₃)	Sherwood	-1.7548	53.4108																							X
UKEAP(NH ₃)	Shetland	-1.0996	60.1420																							X
AURN (Rural), UKEAP(NH ₃)	Sibton	1.4654	52.2943	X																						X
UKEAP(NH ₃)	Silsoe	-0.4147	52.0077																							X
JEP (Aire Valley)	Smeathalls Farm	-1.2256	53.7207							X	X															
AURN (Rural)	Somerton	-2.7359	51.0355	X																						
UKEAP(NH ₃)	Sourhope	-2.2105	55.4898																							X
AURN (Urban Centre)	Southampton Centre	-1.3955	50.9085	X	X	X	X	X																		
AURN (Urban Background)	Southend-on-Sea	0.6752	51.5432	X	X	X	X	X																		
AURN (Rural)	St Osyth	1.0486	51.7779	X	X		X																			
UKEAP(NH ₃)	Stanford	0.7388	52.5190																							X
JEP (South Trent Valley)	Stanton	-1.5998	52.7706							X	X	X		X												
JEP (Midlands)	Stile Cop Cemetery	-1.9437	52.7416								X	X														
AURN (Urban Background)	Stockport Shaw Heath	-2.1609	53.4031		X	X	X	X																		
UKEAP(Precip., NH ₃ , SO ₂)	Stoke Ferry	0.5082	52.5601																		X	X	X	C	X	X
AURN (Urban Centre)	Stoke-on-Trent Centre	-2.1759	53.0282	X	X	X	X	X																		
AURN (Remote)	Strathvaich Dam																									
UKEAP(Precip., NO ₂ , NH ₃ , SO ₂)	Strathvaich Dam	-4.7751	57.7345																		X	X	X	C	X	X
AURN (Urban Background)	Sunderland	-1.3792	54.9062			X																				
UKEAP(NH ₃ , SO ₂)	Sutton Bonington	-1.2503	52.8360																				X		X	X
UKEAP(NH ₃)	Tadcaster	-1.3120	53.9035																							X
JEP (Midlands)	Telford Aqueduct	-2.4596	52.6490								X	X														
JEP (Midlands)	Telford School	-2.4713	52.6328								X	X														
UKEAP(NH ₃)	Thetford	0.8591	52.4199																							X
UKEAP(Precip., NO ₂)	Thorganby	-0.9719	53.8767																		X	X				
JEP (North Trent Valley)	Thorney	-0.7156	53.2480							X	X	X	X	X	X											
AURN (Urban Background)	Thurrock	0.3170	51.4771	X	X	X	X	X																		
UKEAP(NH ₃)	Thursley Common	-0.6987	51.1551																							X
UKEAP(NH ₃)	Tummel	-4.0528	56.7248																							X
UKEAP(Precip., NO ₂)	Tycanol Wood	-4.7781	51.9928																		X	X				
UKEAP(SO ₂)	Wakefield 24	-	-																				X			
AURN (Urban Background)	Walsall Alumwell	-2.0103	52.5825		X																					
AURN (Suburban)	Walsall Willenhall	-2.0325	52.6086		X																					
UKEAP(Precip., NO ₂ , NH ₃)	Wardlow Hay Cop	-1.7346	53.2597																		X	X				X
UKEAP(SO ₂)	Waunfawr 1	-	-																				X			
UKEAP(NH ₃)	Wem Moss	-2.7836	52.9032																							X

Network group	Site name	Longitude	Latitude	Network																						
				AURN						JEP					Particle			UKEAP								
				O ₃ (hourly)	NO/NO ₂ /NOx (hourly)	SO ₂ (hourly)	CO (hourly)	PM ₁₀ (hourly)	PM _{2.5} (hourly)	O ₃ (hourly)	NO/NO ₂ /NOx (hourly)	SO ₂ (hourly)	PM ₁₀ (hourly)	Met (hourly)	Particle Number (hourly)	SMPS (hourly)	Partisol Filter (daily)	NO ₃ (hourly)	EC/OC (hourly)	Precipitation (daily, bulk)	Precipitation (fortnightly, monthly)	NO ₂ (monthly)	SO ₂ (fortnightly)	SO ₄ (daily)	HNO ₃ denuder (monthly)	NH ₃ (monthly)
JEP (Aire Valley)	West Bank	-1.0559	53.7177								X															
AURN (Urban Background)	West London	-0.2008	51.4943	X		X																				
JEP (Thames Estuary)	West Thurrock	0.2877	51.4678								X	X														
UKEAP(NH ₃)	Westhay Moor	-2.7800	51.1921																							X
JEP (South Trent Valley)	Weston on Trent	-1.3957	52.8461							X	X	X		X												
AURN (Rural)	Weybourne	1.1216	52.9505	X																						
UKEAP(Precip., NO ₂)	Whiteadder	-3.5369	55.8617																		X	X				
AURN (Rural)	Wicken Fen	0.2907	52.2987	X	X	X																				
AURN (Urban Background)	Wirral Tranmere	-3.0220	53.3719	X	X	X	X	X																		
UKEAP(Precip.)	Woburn	-0.5953	52.0144																		X	X				
AURN (Urban Centre)	Wolverhampton Centre	-2.1284	52.5878	X	X	X	X	X																		
UKEAP(NH ₃)	Wytham Woods	-1.3449	51.7711																							X
AURN (Rural)	Yarner Wood																									
UKEAP(Precip., NO ₂ , SO ₂ , NH ₃)		-3.7167	50.5971	X																	X	X	X	X	X	X

Notes: (1) Networks: AURN = Automatic Urban Rural Network; JEP = Joint Environment Programme; UKEAP = UK Eutrophying and Acidifying atmospheric Pollutants; (2) Component networks of the UKEAP monitoring programme: NH₃ = Ammonia; NO₂ = Nitrogen Dioxide diffusion tube; Precip. = Precipitation composition; SO₂ = Rural Sulphur Dioxide.

Appendix 4: Model performance metrics

Evaluation of model performance through statistical metrics focuses on measures that compare a set of N predicted concentrations P_i with their counterpart observed concentrations O_i , where i refers to a given time and/or location. Standard metrics used for air quality model performance evaluation are detailed in numerous papers (for example, Chemel *et al.* 2010, Dennis *et al.* 2010 and references therein).

The means of N predictions and observations are defined as:

$$P_{\text{mean}} = \frac{1}{N} \sum_{i=1}^N P_i \quad \text{and} \quad O_{\text{mean}} = \frac{1}{N} \sum_{i=1}^N O_i \quad \text{respectively.}$$

The standard deviations of N predictions and observations are defined as:

$$\sigma_P = \sqrt{\frac{1}{N} \sum_{i=1}^N (P_i - P_{\text{mean}})^2} \quad \text{and} \quad \sigma_O = \sqrt{\frac{1}{N} \sum_{i=1}^N (O_i - O_{\text{mean}})^2} \quad \text{respectively.}$$

The variables a , b , c , and d used to calculate the categorical statistics A , B , H , and FAR represent:

- all the exceedances that did not occur
- exceedances that did occur
- exceedances that were not predicted and not observed, and
- exceedances that were not predicted but observed, respectively.

- Accuracy (no unit, in %):

$$Accuracy = \frac{b+c}{a+b+c+d} \times 100$$

- Bias (no unit):

$$Bias = \frac{a+b}{b+d}$$

- Correlation coefficient (no units):

$$Correlation\ Coefficient = \frac{1}{\sigma_P \sigma_O} \sum_{i=1}^N (P_i - P_{\text{mean}})(O_i - O_{\text{mean}})$$

- Factor of Exceedence (no unit, range (-50,50)%):

$$Factor\ of\ Exceedence = \left[\left(\frac{1}{N} \sum_{i=1}^N i \cdot I(P_i > O_i) \right) - 0.5 \right] \times 100$$

5. Fraction of predictions within a factor of two of observations (no unit, %):

$$\text{Fraction of Prediction} = \left[\frac{1}{N} \sum_{i=1}^N i | (0.5 \leq \frac{P_i}{O_i} \leq 2) | \right] \times 100$$

6. False Alarm Ratio (no unit, in %):

$$\text{False Alarm Ratio} = \frac{a}{a+b} \times 100$$

7. Fractional Bias (no unit, range (-2,2)):

$$\text{Fractional Bias} = \sum_{i=1}^N (P_i - O_i) / \sum_{i=1}^N [(P_i + O_i)/2]$$

8. Fractional Error (no unit, range (0,2)):

$$\text{Fractional Error} = \sum_{i=1}^N |P_i - O_i| / \sum_{i=1}^N [(P_i + O_i)/2]$$

9. Hit Rate (no unit, in %):

$$\text{Hit Rate} = \frac{b}{b+d} \times 100$$

10. Index of Agreement (no unit, range (0,1)):

$$\text{Index of Agreement} = 1 - \frac{\sum_{i=1}^N (P_i - O_i)^2}{\sum_{i=1}^N [|P_i - P_{\text{mean}}| + |O_i - O_{\text{mean}}|]^2}$$

11. Mean Bias (in unit of concentration):

$$\text{Mean Bias} = \frac{1}{N} \sum_{i=1}^N (P_i - O_i)$$

12. Mean Error (in unit of concentration):

$$\text{Mean Error} = \frac{1}{N} \sum_{i=1}^N |P_i - O_i|$$

13. Mean Fractional Bias (no unit, range (-200%, 200%)):

$$\text{Mean Fractional Bias} = \sum_{i=1}^N \{(P_i - O_i)/[(P_i + O_i)/2]\} \times 100$$

14. Mean Fractional Error (no unit, range (0, 200%)):

$$\text{Mean Fractional Error} = \sum_{i=1}^N \{|P_i - O_i|/[(P_i + O_i)/2]\} \times 100$$

15. Mean Normalised Bias (no unit, range (-100%, ∞)):

$$\text{Mean Normalised Bias} = \frac{1}{N} \sum_{i=1}^N \left[\frac{P_i - O_i}{O_i} \right] \times 100$$

16. Mean Normalised Error (no unit, in %):

$$\text{Mean Normalised Error} = \frac{1}{N} \sum_{i=1}^N \left[\frac{|P_i - O_i|}{O_i} \right] \times 100$$

17. Normalised Mean Bias (no unit, range (-1, ∞)):

$$\text{Normalised Mean Bias} = \frac{\sum_{i=1}^N [P_i - O_i]}{\sum_{i=1}^N O_i}$$

18. Root Mean Square Error (in unit of concentration):

$$\text{Root Mean Square Error} = \sqrt{\frac{1}{N} \sum_{i=1}^N (P_i - O_i)^2}$$

19. Skill Variance (no units):

$$\text{Skill Variance} = \frac{\sigma_p}{\sigma_o}$$

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