Options for air quality research: monitoring, modelling and integration

Chief Scientist’s Group Report

December 2023

Version: SC220033

We are the Environment Agency. We protect and improve the environment.

We help people and wildlife adapt to climate change and reduce its impacts, including flooding, drought, sea level rise and coastal erosion.

We improve the quality of our water, land and air by tackling pollution. We work with businesses to help them comply with environmental regulations. A healthy and diverse environment enhances people's lives and contributes to economic growth.

We can't do this alone. We work as part of the Defra group (Department for Environment, Food & Rural Affairs), with the rest of government, local councils, businesses, civil society groups and local communities to create a better place for people and wildlife.

Published by:

Environment Agency
Horizon House, Deanery Road,
Bristol BS1 5AH

www.gov.uk/environment-agency

Further copies of this report are available from our publications catalogue: www.gov.uk/government/publications or our National Customer Contact Centre: 03708 506 506

Email: research@environment-agency.gov.uk

Author(s):
Frances Marshall, Jenny Stocker,
Tim Williamson, Ben Marner, James O'Neill, Victoria Hamilton, David Carruthers, Christina Hood

Keywords:
Monitoring, modelling, integration, assessments.

Research contractor:
Air Quality Consultants Ltd, 23 Coldharbour Road, Bristol, BS6 7JT, 0117 974 1086

Environment Agency's Project Team:
Vera Lucia Barbosa, Rob Kinnersley, Philippa Douglas

Project number:
SC220033

Citation:
Environment Agency (2023), Options for air quality research: monitoring, modelling and integration. Environment Agency, Bristol.

Research at the Environment Agency

Scientific research and analysis underpins everything the Environment Agency does. It helps us to understand and manage the environment effectively. Our own experts work with leading scientific organisations, universities and other parts of the Defra group to bring the best knowledge to bear on the environmental problems that we face now and in the future. Our scientific work is published as summaries and reports, freely available to all.

This report is the result of research commissioned by the Environment Agency's Chief Scientist's Group.

You can find out more about our current science programmes at: https://www.gov.uk/government/organisations/environment-agency/about/research

If you have any comments or questions about this report or the Environment Agency's other scientific work, please contact research@environment-agency.gov.uk.

Dr Robert Bradburne
Chief Scientist

Contents

Acknowledgements

The authors would like to thank the following individuals for their participation in the workshops and individual discussions, and for reviewing sections of the report relevant to their area of expertise:

Dr James Allan (University of Manchester)

Dr David Carruthers (Cambridge Environmental Research Consultants)

Dr Ka Lok Chan (Rutherford Appleton Laboratory)

Chris Connor (Scottish Environment Protection Agency)

Dr Chris Dore (Aether)

Dr Tom Gardiner (National Physical Laboratory)

Professor Roy Harrison (University of Birmingham)

Dr Brian Kerridge (Rutherford Appleton Laboratory)

Dr Barry Latter (Rutherford Appleton Laboratory)

Dr Richard Maggs (Bureau Veritas)

Dr Nick Martin (National Physical Laboratory)

Steve Moorcroft (Air Quality Consultants)

Dr Eiko Nemitz (UK Centre for Ecology and Hydrology)

Amy Stidworthy (Cambridge Environmental Research Consultants)

Dr Gareth Thomas (Rutherford Appleton Laboratory)

Dr Massimo Vieno (UK Centre for Ecology and Hydrology)

Dr Huw Woodward (Imperial College London)

We also thank the project steering committee, which comprised of air quality experts from across the Environment Agency.

Executive summary

Overview

Air quality is a major environmental factor affecting human and ecosystem health in both urban and rural situations. The sources of air pollution that contribute to poor air quality change over time, and assessment methods have evolved accordingly. The Environment Agency's assessment capability, which uses modelling and monitoring techniques, must also adapt to take such changes into account.

This project reviews monitoring, modelling and integration techniques that are currently used within air quality assessments, and identifies whether additional techniques could be introduced that would lead to more accurate and defensible assessments.

The project comprises 4 main stages:

- **Task 1** – gathering preliminary information on the Environment Agency's assessment needs, based on an initial discussion with an Environment Agency project steering committee
- **Task 2** – synthesising information from leading experts in the field of air quality through a series of workshops and individual discussions to produce a comprehensive list of methods that may be of interest to the Environment Agency
- **Task 3** – defining a shortlist of methods, based on a discussion of the comprehensive list with the Environment Agency project steering committee
- **Task 4** – carrying out a literature review of each shortlisted method, considering its usefulness and practical applications to the Environment Agency

Outcomes

Following the workshops and discussions in Task 2, several potential monitoring, modelling and integration methods were identified. The value of each method was discussed with the Environment Agency project steering committee as part of Task 3, and a shortlist of 21 methods carried forward to Task 4.

As well as exploring each method further in the context of air quality, the review identified any limitations and improvements required to maximise the potential of each method, including the need for additional guidance to ensure that the method is fit for purpose for air quality assessments.

Following the literature review, the project provided the Environment Agency with advice on the:

- current status of each shortlisted method, in terms of its readiness for applications, the usage of the method in air quality assessments and the level of expertise required to apply the method
- accuracy of monitoring techniques reviewed as part of Task 4
- relevance of each shortlisted method to the Environment Agency's requirements, including both current areas of involvement and future needs

Finally, the project reviewed the suitability of the identified shortlisted methods for 6 case studies, covering specific pollutants (ammonia and nitrogen oxides from combustion), and polluted environments that the Environment Agency is currently required to assess. The project also attempted to determine whether there are any better approaches that could be applied in these circumstances based on the shortlisted methods.

The main findings of the project are summarised in the table below as options for research.

Topic	Finding
Monitoring methods	There are a number of monitoring methods available which are suitable for a range of pollutants. The different methods offer varying temporal resolutions, spatial coverages and purchase costs. Each method is, however, associated with its own inherent uncertainty, and its application does, therefore, require careful consideration to ensure that the technique is fit for purpose. The rise in low-cost sensors (LCS) could potentially expand geographical coverage and enable access to monitoring equipment for the wider population. However, it has also highlighted the importance of equipment certification and the need for guidance to be followed when using any monitoring device.
Modelling methods	Models can potentially be developed to assess the impact of new activities and fuels. Models are available that can represent processes at small and large temporal and spatial scales. Joining one model with another, or with measurements, also allows a range of scales to be accounted for. Although underlying model formulations should be verified by model developers, the results of model applications are highly dependent on correct model configuration. Model users should be encouraged to compare results with measurements, and/or to provide explanations for model results.
Integrated monitoring and modelling methods	Measurements are commonly used as inputs to models, for calibration or as boundary conditions. In general, the more complex methods for integrating modelling and monitoring are not widely available for standard air quality assessments. However, some integration techniques (for example, data assimilation, machine learning) are well established in fields other than air quality. With the increasing availability of air quality measurement data sets, reviewing the applicability of these techniques to air quality applications may benefit the air quality practitioner community.

Project options for research are summarised in the table below.

Topic	Option for research
Guidance	There are existing modelling and monitoring guidance documents that have been generated for different groups, committees and users. Consolidating these documents with those written by the Environment Agency/Department for Environment, Food and Rural Affairs (Defra) into a central place would streamline air quality assessments. Equally, the review has highlighted several areas, such as deposition modelling and low-cost sensors, where additional guidance could be beneficial to ensure they are applied correctly.
Protocols	A coordinated approach to air quality assessments of common, complex situations, such as industrial clusters, could be facilitated by establishing protocols, including preparing guidance and creating steering groups.
Monitoring networks	Extensions to the national monitoring networks, such as the National Ammonia Monitoring Network (NAMN), could assist with documenting concentrations in areas that are currently sparsely covered, including coastal areas. As additional monitoring devices are certified, there is also the potential to complement existing monitoring networks with alternative technologies, although this would depend on the requirements of the monitoring network. Investment in lower accuracy monitors to map the state of pollutants across large geographical areas could help with targeted placement of higher accuracy monitors.
Tool suitability	A comprehensive set of monitoring and modelling tools exists, but all tools have limitations, for instance in terms of their applicability over geographic area and timescales. The information presented in this study could be summarised to inform the air quality community about tool suitability for a range of common air quality assessments. It is important to keep such guidance updated to reflect current tool capabilities.
Database development	The Environment Agency, alongside other regulatory bodies, holds an extensive catalogue of monitoring data, which could be a valuable resource for the research community, particularly with respect to cumulative pollutant exposure and potential compliance issues. Establishing a secure and robust database, in collaboration with other bodies, and subsequently a relationship as a data provider, could be highly beneficial and an option to consider.
Inventories	To ensure that the modelling techniques used within air quality assessments are robust and defensible, periodic reviews into emissions databases, particularly with respect to new fuels and sources would be useful. Validating emissions inventories, including emissions measurements, could also help in quantifying impacts in complex environments.

1. Introduction

The role of the Environment Agency is to protect and improve the environment and places for people, and to be a champion of sustainable development. This includes addressing pollution issues in relation to the quality of the air, land and water that it is responsible for. In the context of emissions to air, the Environment Agency's current responsibilities and tasks include:

- regulatory responsibilities, including:
    - ensuring certain permitted industrial processes and waste management activities prevent, or where that is not possible, minimise emissions that have the potential to cause pollution or harm to human health
    - radioactive releases
- operating air quality monitoring networks, in partnership with the Department for Environment, Food and Rural Affairs (Defra) across the UK
- operating the air quality major incidents service to support other Category 1 responders as required by the Civil Contingencies Act

There are a wide range of air quality modelling and monitoring tools available to the Environment Agency to help with the responsibilities and tasks described above, many of which are commonly applied in air quality assessments. In some cases, modelling and monitoring methods are used independently of one another. However, the methods can also be integrated to enhance the utility of the tools. The complexity of the tools ranges from simple methods that can be carried out by non-specialist users, through to comprehensive methods that require specialised understanding of air quality monitoring and modelling. Several aspects need to be considered to identify a 'fit-for-purpose' technique, including resources, technological capability, temporal and spatial demands, and the required level of accuracy.

The Environment Agency is interested in assessment methods for the following polluted environments, using currently available tools and techniques:

- releases in complex built urban and industrial environments, where there are morphological factors, such as buildings that influence the dispersion properties of the plume, and where there are potentially multiple other nearby sources that contribute to total concentrations
- in-combination impacts from multiple sources of pollution, such as industrial clusters, and human health impacts arising from cumulative pollutant exposure to multiple different species at varying thresholds

Additionally, the air quality landscape is evolving, and in future the Environment Agency may also be required to carry out air quality assessments for:

- new industrial activities, such as carbon capture, utilisation and storage (CCUS) that may come forward because of societal and political shifts
- new fuels, such as ammonia (NH_3) and hydrogen (H_2) that may become more prominent as industries and applications adopt the use of cleaner, greener fuels

The Environment Agency needs to be equipped with a range of fit-for-purpose tools that reflect the current and future air quality landscape to ensure air quality impact assessments for ecosystems and human health are defendable. This review considers 21 current and emerging methods in the air quality monitoring, modelling and integration sectors that have the potential to enhance the Environment Agency's assessment capabilities. These 21 shortlisted methods have been developed through discussions with air quality experts and an Environment Agency project steering committee.

In assessing the available methods, the review also attempts to highlight the limitations associated with each approach, and aims to outline options for improvements and/or further research that may be necessary to maximise the potential of each approach.

1.1. Project objectives

Specific objectives of the project are to:

- review present and likely future air quality assessment needs and what they will require with respect to monitoring, modelling and integration techniques, including consideration of spatio-temporal scales, representativeness, resolving power and statistical rigour. The future assessment needs will take account of the changing emissions landscape arising from, for instance, pathways to net zero
- evaluate the factors that limit delivery of present and likely future air quality assessment needs and identify what is needed to overcome them
- identify state-of-the-art and developing areas in air quality monitoring and modelling, including new opportunities to exploit hierarchical sensor webs, satellite and other remote sensing platforms, and new factors affecting model developments, such as machine learning (ML) and cloud computing
- review the state-of-the-art approaches to the integration of monitoring and modelled data, which may come from multiple sources and models at a range of spatial and temporal scales with differing levels of statistical uncertainty
- review methods available to optimise monitoring network design to provide fit-for-purpose coverage, resolution, confidence limits and optimal resource use
- identify where new techniques have the potential to enable or improve assessment approaches, and what steps or additional work would be required to realise that potential
- review monitoring and modelling methods specific to assessing emissions arising from new technologies emerging, for instance, from pathways to net zero (for example, amines and their degradation products arising during carbon capture, utilisation and storage (CCUS)
- review the state of readiness for each method, including whether additional research or investigation is required to realise the method's full potential
- consider the accuracy of current monitoring technologies, including any mismatch between current capabilities and any shortfall relative to present and future Environment Agency needs

It should be noted that, while this report endeavours to provide a high-level summary of a variety of practical methods that may be of value to the Environment Agency, it is not intended to be an extensive or exhaustive review or to provide specific recommendations for future investment.

1.2. Report structure

To help with the evaluation, the current status of each method has been considered (section 2.1), as well as identifying the Environment Agency's regulatory areas of responsibility or interest to which each method might be applicable (section 2.2). Finally, the review has considered a series of common circumstances that the Environment Agency encounters, and suggests how an individual method, or combination of methods, might be of value (section 2.3).

The main findings and options for potential future research from the project, grouped according to the common themes of the review, are provided in section 3.

Section 4 provides some concluding remarks and considers the next steps for the project, including reference to a separate parallel project that identifies the drivers of future changes to air quality (SC220032/R) (Environment Agency, 2023a).

Details of the project approach are summarised in Appendix A1, while Appendix A2 provides the comprehensive list of methods from which the shortlist was derived. Following a review of the comprehensive list with the Environment Agency project steering committee, several methods were not progressed; a high-level summary of these methods is provided in Appendix A3. Appendix A4 summarises the conclusions of the literature review.

Current status

To determine the current status of each method, the project has considered the state of readiness, the usage of the method for air quality applications, and the level of expertise required to apply the method. In the case of monitoring techniques, the accuracy of each technique for measuring different pollutants has also been considered, alongside any gaps relative to current and future needs.

A classification of the current status for each method is provided in Table 1, while suitability for monitoring is presented in Table 2.

Assignment to Environment Agency relevance

The relevance of each shortlisted method to the Environment Agency's requirements, current areas of involvement and future needs has been considered.

A summary of relevance for each method is provided in Table 4.

Applicability of methods to certain Environment Agency situations

To assess the suitability of the identified shortlisted methods, a high-level literature review was carried out. The conclusions of the literature review are provided in Appendix A4, and aim to answer the following questions:

1. How much further exploration or guidance is required to enable the Environment Agency to adopt the method?
2. Does the method require additional development to ensure that it is fit for purpose?
3. What are the limitations of the method, and how might this affect the Environment Agency?
4. Is it possible to indicate the level of uncertainty in the assessment method?

Following the literature review, section 2.3 considers the suitability of the identified shortlisted methods for the following topics and Environment Agency applications:

- ammonia
- nitrogen oxides (NOx) from combustion
- cumulative pollutant exposure
- intensive farming
- industrial clusters
- built environments

Section 2.3 also seeks to determine how the method might improve the Environment Agency's current capability.

2. Detailed review of shortlisted methods

This section summarises the:

- current status of each shortlisted method
- accuracy of each technique for measuring different pollutants
- relevance to the Environment Agency of each shortlisted method
- suitability of the methods for certain topics and Environment Agency applications

2.1. Current status of shortlisted methods

Table 1 presents the state of readiness for each method. An explanation for each assignment is as follows:

- State of readiness:
    - **Readily available** – no further research or guidance is required to adopt this method into air quality assessments.
    - **Prototype** – the method is undergoing field testing and requires additional guidance for implementation.
    - **Research** – the method is still under development.
- Usage:
    - **Well established** – the method is widely cited in the literature. Where appropriate, the method has been certified to recognised standards.
    - **Case studies available** – examples of the method’s application in air quality assessments are available in the literature.
    - **Few applications** – there are limited examples in the literature.
- Level of expertise:
    - **Low** – the method does not need any prior understanding of air quality assessments. This does not, however, guarantee that the method will be applied correctly by non-specialists.
    - **High** – expertise is required to apply the method to air quality assessments, since an extensive understanding is required to formulate inputs, operate the method and process outputs.

Table 1: Current status of shortlisted methods

Item	Method	State of readiness	Usage	Level of expertise
1	Gaussian plume modelling	Readily available	Well established	Low - High
2	Lagrangian Gaussian puff modelling	Readily available	Well established	Low - High
3	Lagrangian particle modelling	Readily available	Well established	Low - High
4	Grid-based Eulerian models	Readily available	Well established	High
5	Computational fluid dynamics modelling	Readily available	Well established	High
6	Modelling of non-linear processes: complex chemistry/radioactivity	Readily available	Well established	Low - High
7	Dry and wet deposition modelling	Readily available	Well established	Low - High
8	Complex terrain wind field modelling	Readily available	Well established	Low - High
9	Nested/coupled modelling systems	Prototype	Case studies available	High
10	Ensemble modelling	Prototype	Case studies available	Low - High
11	Passive samplers	Readily available	Well established	Low - High
12	Low-cost sensors	Readily available	Case studies available	Low - High
13	Reference monitors	Readily available	Well established	High
14	Urban supersites	Readily available	Case studies available	High
15	Mobile air quality monitoring	Prototype	Case studies available	Low - High
16	Ground-based remote sensing measurements	Research	Few applications	High
17	Siting of monitors	Readily available	Well established	Low - High
18	Hierarchical networks	Research	Few applications	High
19	Data assimilation	Readily available	Case studies available	Low - High
20	Machine learning/deep learning	Research	Case studies available	High
21	Satellite measurements	Readily available	Case studies available	High

Table 2 presents the accuracy of the monitoring techniques discussed in sections A4.11 to A4.21 for a range of commonly encountered pollutants. An explanation for each assignment is as follows:

- **High** – the technique meets reference equivalent standards.
- **Medium** – the technique meets indicative standards.
- **Low** – the method is associated with large uncertainties.
- Dash (**-**) – the method is not available for that pollutant.

Table 2: Accuracy of monitoring methods for different pollutants

Method	**Pollutant**				
	Nitrogen dioxide (NO_2)	**Particulate matter (PM_{10} and $PM_{2.5}$)**	**Volatile organic compounds (VOCs)**	**Ammonia (NH_3)**	**Sulphur dioxide (SO_2)**
11 – Passive samplers					
Diffusion tubes	**Medium**	**-**	**Medium**	**Medium**	**Medium**
Filtered diffusion tubes	**High**	**-**	**-**	**-**	**-**
DEnuder for Long-Term Atmospheric sampling (DELTA)	**-**	**-**	**-**	**High**	**High**
Adapted Low-cost Passive High Absorption samplers	**-**	**-**	**-**	**Medium**	**-**
12 – Low-cost sensors					
Optical counters	**-**	**Low**	**-**	**-**	**-**
Electrochemical sensors	**Low**	**-**	**Low**	**Low**	**Low**
Metal oxide semiconductors	**-**	**-**	**Low**	**-**	**-**
Flame ionisation detectors	**-**	**-**	**Low**	**-**	**-**
13 – Reference monitors					
Chemiluminescence monitors	**High**	**-**	**-**	**Low**	**High**
Ultra-violet fluorescence monitors	**-**	**-**	**-**	**-**	**High**
Gravimetric instruments	**-**	**High**	**-**	**-**	**-**
Tapered element oscillating microbalances	**-**	**High**	**-**	**-**	**-**
Optical particle size	**-**	**High**	**-**	**-**	**-**

Method	**Pollutant**				
	Nitrogen dioxide (NO_2)	**Particulate matter (PM_{10} and $PM_{2.5}$)**	**Volatile organic compounds (VOCs)**	**Ammonia (NH_3)**	**Sulphur dioxide (SO_2)**
spectrometers					
Gas chromatography	**-**	**-**	**High**	**-**	**-**
16 – Ground-based remote sensors					
Active	**Medium**	**Medium**	**Medium**	**Medium**	**Medium**
Passive	**Low**	**Low**	**Low**	**Low**	**Low**
21 – Satellites [a]					
Short wavelengths	**Low**	**Low**	**Low (for example, formaldehyde)**	**-**	**Low**
Infrared wavelengths	**-**	**Low**	**Low (for example, methanol)**	**Low**	**-**

[a] Satellites require a modelling component to enable concentrations to be inferred from measurements of shortwave and longwave radiation and so they are an integration technique rather than purely a monitoring technique.

2.2. Relevance of shortlisted methods to the Environment Agency’s requirements

Table 4 reviews each shortlisted method in the context of the Environment Agency’s regulatory requirements, current areas of involvement and future needs. The symbols used to describe relevance are described here in Table 3.

Table 3: Classification used to assign Environment Agency relevance

Symbol	Description
✓	The method is appropriate for calculating regulatory or statutory air quality metrics.
(✓)	The method can be used to assess air quality but is not suitable for directly calculating regulatory or statutory air quality metrics.
✓*	The method is appropriate for calculating regulatory or statutory air quality metrics if the equipment meets minimum certification requirements. This only applies to monitoring methods.
?	It is not possible to definitively state whether this method could be used for the specified activity. For example, in the case of new fuels or new industrial activities, the scope of the requirement is not currently known, and measurement equipment has the potential to be developed in the future to measure emerging pollutants.
N/A	The method cannot be used in isolation for air quality assessments.
	Where the cell is blank, the method is not relevant to the particular application.

Table 4: Relevance of shortlisted methods to the Environment Agency's requirements

Item	**Method**	**Regulatory responsibilities**					**Other**				**Air quality monitoring networks**	**Accidental releases**
		A1 installations	**Intensive farming**	**Waste activities**	**Medium combustion plant**	**Radioactive releases**	**New industrial activities**	**New fuels**	**Built environments**	**Cumulative impacts**		
1	Gaussian plume modelling	✓	✓	✓	✓	✓	?	?	✓	✓		✓
2	Lagrangian Gaussian puff modelling	✓				✓	?	?				✓
3	Lagrangian particle modelling	✓	✓	✓	✓	✓	?	?	✓	✓		✓
4	Grid-based Eulerian models	✓				✓	✓	✓		✓		✓
5	Computational fluid dynamics modelling	(✓)	(✓)	(✓)	(✓)		?	?	(✓)	?		(✓)
6	Modelling of non-linear processes:	N/A – the air quality models described above account for these processes in varying levels of detail.										

Item	**Method**	**Regulatory responsibilities**					**Other**				**Air quality monitoring networks**	**Accidental releases**
		A1 installations	**Intensive farming**	**Waste activities**	**Medium combustion plant**	**Radioactive releases**	**New industrial activities**	**New fuels**	**Built environments**	**Cumulative impacts**		
	complex chemistry/ radioactivity											
7	Dry and wet deposition modelling	N/A – the air quality models described above account for these processes in varying levels of detail.										
8	Complex terrain wind field modelling	N/A – the air quality models described above account for these processes in varying levels of detail.										
9	Nested/coupled modelling systems	✓	✓	✓	✓	✓	?	?	✓	✓		✓
10	Ensemble modelling	✓	✓	✓	✓	✓	?	?	✓	✓		✓
11	Passive samplers	✓	✓	✓	✓	?	?	?	✓	✓	✓	
12	Low-cost sensors	✓*	✓*	✓*	✓*	?	?	?	✓*	✓*	✓	✓*

Item	Method	Regulatory responsibilities					Other				Air quality monitoring networks	Accidental releases
		A1 installations	Intensive farming	Waste activities	Medium combustion plant	Radioactive releases	New industrial activities	New fuels	Built environments	Cumulative impacts		
13	Reference monitors	✓	✓	✓	✓		?	?	✓	✓	✓	✓*
14	Urban supersites						?	?	?	?	✓	
15	Mobile air quality monitoring	(✓)	(✓)	(✓)	(✓)	?	?	?	(✓)	(✓)	✓	✓
16	Ground-based remote sensing measurements	(✓)	(✓)	(✓)	(✓)		?	?	(✓)	(✓)		?
17	Siting of monitors and network optimisation	N/A – this is not an air quality assessment method. However, it can be an important step in carrying out air quality assessments. It often uses modelling to inform the siting of monitors and so involves integration.										
18	Hierarchical networks	✓*	✓*	✓*	✓*	?	?	?	✓*	✓*	✓	✓*

Item	**Method**	**Regulatory responsibilities**					**Other**				**Air quality monitoring networks**	**Accidental releases**
		A1 installations	**Intensive farming**	**Waste activities**	**Medium combustion plant**	**Radioactive releases**	**New industrial activities**	**New fuels**	**Built environments**	**Cumulative impacts**		
19	Data assimilation	N/A – needs to be carried out in combination with other modelling and/or monitoring methods.										
20	Machine learning/ deep learning	N/A – needs to be carried out in combination with other modelling and/or monitoring methods.										
21	Satellite measurements	(✓)	(✓)	(✓)			?	?			✓	✓

2.3. Suitability of the methods to Environment Agency applications

This section reviews the conclusions of the high-level literature review of the shortlisted methods in the context of some the Environment Agency's current and future regulatory requirements, using 6 case studies.

Ammonia

Ammonia is important from a human health perspective since it acts as a precursor to the formation of secondary particulate matter. It is also important from an ecological perspective, because deposition of nitrogen can lead to changes in nitrogen loadings (nutrient nitrogen) and accumulation of nitrogen on flora (acid nitrogen deposition) (The Royal Society, 2018). Ammonia emissions are regulated under the National Emissions Ceiling Regulations (NECR) (European Commission, 2016). However, as there are no statutory human health ammonia limits, air quality assessment of ammonia is currently associated with impacts on habitats.

Gaseous ammonia is emitted to the atmosphere primarily as a result of agricultural activities, which contributed 87% of total ammonia emissions in the UK in 2021. The remainder is associated with waste (3% in the UK in 2021) and other diffuse sources such as those from sewage. Other diffuse sources are from the use of ammonia in selective catalytic reduction technology in vehicles (2% in the UK in 2021), and from industry and biomass burning (Defra, 2023a). There are also emerging sources of ammonia emissions that may need considering further, including anaerobic digestors, the movement of agricultural waste, and fugitive emissions from ammonia fuel usage and carbon capture, utilisation and storage (CCUS).

The lifetime of ammonia in the atmosphere is relatively short (hours to days). This is because it is readily deposited by both dry and wet processes, and it also reacts with nitric acid and sulphuric acid, formed from the oxidation of NOx and SO_2, to generate secondary particulates.

Currently, monthly measurements of gaseous ammonia are carried out at ~72 sites across the UK as part of the National Ammonia Monitoring Network (NAMN) (Defra, 2023b). The network uses DEnuder for Long-Term Atmospheric (DELTA) active diffusion samplers and a secondary network of Adapted Low-cost Passive High-Absorption (ALPHA) samplers. It is not, however, practical to directly measure total nitrogen deposition, which is the sum of both wet and dry deposition processes. A small number (~27) of sites within the NAMN measure wet deposition in the form of particulate ammonium (NH_4^+), but dry deposition is typically assessed using models rather than monitors.

The original purpose of the NAMN was to observe changes in the agricultural sector and to verify compliance with international targets and agreements. Consequently, NAMN monitors are typically situated in 'background' locations, with only one location (London, Cromwell Road) being described as 'roadside'. This demonstrates a notable absence of monitors in urban settings. There are also very few examples of comprehensive monitoring studies for ammonia. An extensive monitoring study of traffic-related ammonia on Ashdown Forest Special Area of Conservation (SAC) was carried out by Air Quality Consultants Ltd (AQC) between 2014 and 2016 (Air Quality Consultants Ltd, 2018). The nature of the monitoring network enabled spatial and temporal trends to be deciphered, which may apply beyond Ashdown Forest and could facilitate more accurate modelling in the future.

A more complete understanding of ammonia, in terms of its sources, processes and effects, does, therefore, require the implementation of additional monitoring networks across the UK. Establishing suitable monitors is, however, compounded by the limited technology available, particularly in the case of low-cost sensors (LCS) when concentrations are low. An emerging requirement for monitoring (and modelling) is the need to assess the effect of tree shelter belts in abating plumes of ammonia from agriculture, including Environment Agency-regulated intensive pig and poultry sites, and potentially from beef and dairy cattle. In the future, monitors using nanomaterials that can respond in real-time may become mainstream. However, these products are still relatively undeveloped. With respect to measuring processes associated with ecosystems, such as wet deposition, cavity ringdown spectrometers have been shown to be less efficient than diffusive samplers, owing to the effects of cross-interference from water vapour (Martin and others, 2016). The ongoing benchmarking of ammonia measurements as part of the Integrated Research Observation System for Clean Air (OSCA) (UK Research and Innovation, 2019) will, however, help in widening the technological field. Phase 1 was recently completed, which included using the University of Manchester supersite to validate measurements. There is also the opportunity for satellite monitoring to help further with measurements of ammonia, including the Meteosat Third Generation (MTG) geostationary satellites, which will comprise an infrared (IR) spectrometer for detecting ammonia. While the on-board equipment is comparable to satellites in polar orbit, the MTG satellites will have a smaller field of view (approximately 4 x 4km), enabling them to focus on regions at an hourly resolution. This type of satellite monitoring could enable hotspots to be determined, which could then facilitate the creation of a coordinated ground-level monitoring network using passive or active sampling techniques.

Models are used to calculate the environmental impacts of ammonia at a range of temporal and spatial scales. Current model inventories attribute most ammonia emissions to agricultural sources, which may result in other important sources being overlooked or omitted. Short-range impacts of ammonia on habitats are commonly assessed using Gaussian plume models such as the Atmospheric Dispersion Modelling System (ADMS) and American Meteorological Society and United States Environmental Protection Agency (US EPA) Regulatory Model (AERMOD). These models represent source geometries and emissions characteristics, and can calculate ambient concentration and deposition fluxes; wet deposition fluxes are assumed to be negligible in comparison to dry in the near field (AQTAG, 2011). The relationship between concentrations and dry deposition fluxes, and therefore the increase in nitrogen, is usually assumed to be linear (refer to section A4.7), but at higher concentrations this relationship breaks down. ADMS allows 3 terms of the diffusive component of dry deposition to be modelled: aerodynamic, sub-layer and surface resistance; of these, the first 2 depend on meteorological conditions and the third relates to surface properties and pollutant reactivity. AERMOD also allows for relatively complex approaches to modelling dry deposition, allowing the user to input parameters such as the leaf area index, which is used to determine the surface resistance component of the deposition velocity.

The Dutch Operational model for Priority Substances (OPS) model (van Jaarsveld, 2004), which has been developed for the specific purpose of calculating the deposition of acidifying compounds over the Netherlands at a high spatial resolution, includes the Deposition of Acidifying Compounds (DEPAC) module (van Zanten and others, 2010). DEPAC accounts for the deposition processes modelled in ADMS and AERMOD, but additionally takes a ‘compensation point’ approach, whereby the model accounts for the difference between ambient concentrations and concentrations in the stomata and at the leaf surface. This approach can, in theory, result in conditions where ammonia is released back into the atmosphere. ADMS allows the spatial and temporal variation of deposition velocities to be modelled, which goes some way to representing the dependence of deposition velocity on ground level concentrations. This modelling approach is recommended in Natural Resources Wales’ guidance in relation to modelling the concentration and deposition of ammonia emitted from intensive farming (Natural Resources Wales, 2019). The Joint Nature Conservation Committee (JNCC) is developing the online UK Air Pollution Assessment Service (APAS) to facilitate an integrated approach to UK risk assessment of air pollution effects on ecosystems and statutory reporting requirements. Ammonia concentrations and deposition can be modelled within APAS, which incorporates the ADMS model. The UK Centre for Ecology and Hydrology's (UKCEH) Concentration Based Estimated Deposition (CBED) model generates 5 x 5km resolution maps of wet and dry deposition of reduced and oxidised nitrogen from measured concentrations of atmospheric pollutants, including ammonia, and measured concentrations of ions in precipitation.

Assuming constant deposition velocities for ammonia can be considered a conservative modelling approach in terms of near-field deposition. However, if plume depletion is also modelled, then plume concentrations in the far field may be too low, resulting in under-predictions of far field deposition fluxes. Therefore, care should be taken to ensure that the correct level of detail is modelled when predicting deposition fluxes at sensitive habitats.

Long range pollutant transport and chemical processes associated with ammonia can be modelled using chemical transport models (CTMs), such as the European Monitoring and Evaluation Programme (EMEP) (Simpson and others, 2012). Modelled ammonia concentrations and total nitrogen deposition fluxes (including that due to NO_X) are available to download from UKCEH’s Air Pollution Information System (UKCEH, 2023), at up to 1km resolution.

NOx from combustion

Emissions of NOx arising from the combustion of fossil fuels have been well documented in the literature (Defra, 2023c). NO_X is important as a primary pollutant and has an important role in the generation of secondary pollutants, including O_3 and particulates. Decarbonisation of the energy sector could, however, lead to additional NOx emissions through the combustion of hydrogen as an alternative fuel, as could using ammonia as a low-carbon fuel in the maritime industry. However, currently, the evidence related to the magnitude of emissions associated with these new technologies and fuels is uncertain, with studies suggesting that emissions of NOx from the combustion of hydrogen may be higher than those from combustion of natural gas, owing to increased burn temperatures (Aether, 2023).

Current approaches to recording ambient NO_X and NO_2 concentrations should be suitable for monitoring near new NO_X sources, but may require additional monitoring sites in coastal areas to account for NO_X emissions from ships using ammonia as a fuel. Similarly, in terms of modelling NO_X emissions from new sources, current approaches that account for short- and long-range pollutant dispersion processes should continue to be appropriate.

New or revised model input parameters will be necessary to correctly represent new sources, for instance emission rates of both NO_X and NO_2, and source release properties.

Cumulative (multi-pollutant) exposure

Although many studies have investigated the effects of single pollutants on human health, communities will be exposed to mixtures of pollutants over prolonged periods. The effect of exposure to individual pollutants at high concentrations has been well documented in the literature (Committee on the Medical Effects of Air Pollutants, 2023). However, some studies have shown that multiple substances can lead to synergistic effects, where the effect of combined pollutants is greater than the individual effects (Carpenter and others, 2002).

Each pollutant may have a different entrance pathway, such as through ingestion, inhalation and skin contact; and/or it may reside in the body for different timescales; and/or it may undergo different biological, chemical and physical transformations between source and receptor. The study of cumulative pollutant exposure is, therefore, complex, and depends on the chemical composition of the mixture, the chemical and physical processes that occur between source and receptor, and the nature of the population affected.

As set out in a concurrent project, “Options for air quality research: Drivers of future changes” (Environment Agency, 2023a), if cumulative exposure does manifest as a growing area of concern, the Environment Agency needs to understand how to respond. However, the ability to regulate and manage the potential for cumulative pollutant exposure needs robust evidence of the impacts (human health and environmental) to conclusively quantify the cumulative effect, although this evidence is currently limited. As such, given the wealth of available monitoring data, there is a potential role for the

Environment Agency to act as a data provider to enable health and environmental impacts studies to advance. Establishing a relationship between the Environment Agency and the research community would be critical to maximise the benefits of any transferred data, for example, ensuring the data are for the correct pollutants and from relevant monitoring locations.

Intensive farming

Intensive farming, involving both crops and livestock, refers to maximising agricultural production on a given area of land, using large amounts of labour, capital and resources relative to the land area. Processes and activities associated with intensive farming can lead to emissions of the following pollutants, all of which have the potential to affect air quality:

- ammonia, which partitions into the atmosphere as a result of the application of animal waste, such as slurry and manure, urea, and pesticides onto fields in an attempt to maximise crop yields
- particulate matter, which is emitted directly as well as generated through secondary reactions between ammonia, nitric acid and sulphuric acid, as a result of increased quantities of ammonia present in the atmosphere from intensive farming activities
- volatile organic compounds (VOCs) from greater volumes of livestock production
- bioaerosols, which are particles of biological origin that are suspended in the air (also referred to as ‘organic dust’), which arise from increased animal activity and greater stock density, and are affected by the different growth stages of the animals
- methane, which arises from enteric fermentation as part of the animal’s digestive process, and which is a precursor of ground level ozone formation

Natural Resources Wales (2023) and the Northern Ireland Environment Agency (2017) both have intensive farming guidance online. The Atmospheric Dispersion Modelling Liaison Committee (ADMLC) review of the limitations and uncertainties of modelling pollutant dispersion from non-point sources (Stocker and others, 2016; Stocker and others, 2017) focuses on the dispersion modelling of agricultural and bioaerosol source emissions. The report presents 4 case study applications using ADMS and AERMOD, and includes a good practice guidance flow chart suggesting how best to approach an intensive farm modelling study. In addition to highlighting uncertainty associated with bioaerosol emissions, recommendations from this 2016 study include:

- existing technical guidance documents should be updated to reflect the conclusions of the study
- the model developers of ADMS and AERMOD should seek to develop their building modules to allow for dispersion of non-point sources
- in order to improve and standardise the approach to dispersion modelling of bioaerosol emissions, research into the physical processes that occur when these

pollutants disperse is required. Such research should result in guidance on recommended particle size values, with associated mass fractions and coagulation rates

As far as the authors are aware, these recommendations have not been addressed to date.

A discussion of the methods for measuring and modelling ammonia has been provided earlier in this section. The range and magnitude of bioaerosol emissions from intensive farming is a current research topic (Douglas and others, 2018), with a variety of bacterial and fungal species being released. Particulate matter and methane can be modelled using standard approaches, although again care should be taken when calculating emissions, for example, to ensure that growth cycle temporal variations are modelled.

Intensive farmers, as part of the conditions for their operating permits, are required to annually report their emissions to air; the pollutants considered depend on the farming activity. These emissions are calculated based on emission factors, considering the housing type (determined from in-situ monitoring covering a range of different types) and numbers of animals. It is, therefore, important to ensure that the emissions databases are regularly updated with new data, particularly as practices evolve, and technology associated with housing becomes more advanced.

As part of the natural farming cycle, crops and livestock are rotated across the land. As a result, traditional static monitors may not show the full spatial distribution of pollutants across the land. The deployment of mobile monitors using suitably validated monitoring equipment could enable trends in farming practices to be determined, and trace the movement of emission sources, be it livestock or fertiliser application, across extensive areas of land. Measurements from mobile monitors could be coupled with modelling studies to verify emission inventories, and used to detect peaks in agricultural activities, which may help policymakers. Mobile methods could also be complemented with dense static sensor networks to maximise geographical coverage and to monitor temporal changes through the annual farming cycle.

Industrial clusters

Industrial clusters are geographic areas that comprise several similar or different industries. The government’s current Industrial Strategy is to create a net zero carbon industrial cluster by 2040, and at least one low carbon cluster by 2030 (Department for Business, Energy and Industrial Strategy, 2019). Several industrial clusters currently exist in England, Scotland and Wales, including in Grangemouth, Humberside, Merseyside and South Wales.

Industrial clusters present a number of challenges to air quality regulators, not only because they are commonly powered by fossil fuels and emit a variety of pollutants that may interact with one another, but also as they gradually encroach upon urban areas, the potential for in-combination air quality impacts increases. The pursuit of net-zero industries will also introduce obstacles through the emergence of new sources (such as NOx from hydrogen combustion) and pollutants (such as amines from CCUS technology).

The clustering of industries is advantageous from a monitoring design perspective, since all the emissions will arise from a concentrated area, therefore, plume dispersion patterns will broadly overlap in terms of wind direction, and will interact with the same, or similar, topography. Within the cluster, dispersion would be controlled by factors unique to each source (including dependence on source geometry, for example, point, area, fugitive, and emissions parameters) and by local factors such as the effect of nearby buildings. Chemical processes are also complex in environments where there are multiple pollution sources.

Given the complexities surrounding industrial clusters, an integrated assessment approach is an option for assessing air quality impacts. For example:

- The first step would involve deploying a number of on-site and off-site lower sensitivity monitors (such as low-cost sensors (LCS) or passive samplers) to assess the main pollutants. The high temporal resolution of LCS is a distinct benefit for capturing activities within the cluster or meteorological conditions that lead to elevated concentrations, while the low cost of passive samplers would enable large geographical coverage at relatively low expenditure. The type and siting of the monitors would, however, be governed by: (i) the sensitivity of nearby receptors, such as the proximity of residential areas, sensitive habitats and workplaces; (ii) the prevailing meteorological conditions; (iii) the activities taking place in the cluster, and (iv) the source conditions (such as whether the emission sources were elevated or low-level vents). Deployment of a set of well-placed, reliable monitors would enable an initial reconnaissance of the environment, and provide an initial overview to develop subsequent stages of the assessment.
- In order to complement the primary stage of monitoring, initial modelling would also need to be carried out, which would involve:
    - collating an emissions inventory, including associated source geometries and efflux data
    - performing a modelling study using a Gaussian plume/Lagrangian model to identify probable spatial location of high impacts
    - evaluating the model using data from the primary stage of monitors
- Following the initial stages of monitoring and modelling, a hierarchical network of monitors could be established, the siting of which would be dictated based on the plume dispersion properties:
    - A small number of higher accuracy monitors (such as reference monitors or supersites) could be located in areas where the initial modelling and monitoring suggest that ground level concentrations may be highest, or in certain communities.
    - Additional monitoring could take place with lower accuracy monitors to complement the higher accuracy monitors and maximise the geographical coverage of the network, albeit with reliance on frequent calibrations with the

    higher accuracy monitor. Alternatively, existing monitors from the reconnaissance step could be relocated.
    - If any monitors detect elevated concentrations, a communal mobile monitor, in the form of a drone or van operated by the industrial cluster could be deployed to investigate the causes further.
- The final step would involve refining the initial models, including:
    - reviewing the results of the initial modelling to decide how/if the emissions inventory needs to be reviewed
    - deciding if more complex chemical processes or longer-spatial scales need to be modelled, which may be pollutant dependent. At this stage, it might be beneficial to consider using a coupled system, for example, Gaussian plume model nested within a chemical transport model (CTM)
    - evaluating revised/new modelling outputs with new measurement data to establish whether there is good agreement:
        - If so, continue monitoring, and only repeat modelling when sources change or there are new pollutants of interest.
        - If not, review model inputs again including the emissions inventory. Consider inverse modelling approaches to estimate source emissions.

This approach requires significant resources initially, and some ongoing resources to support monitoring networks. Establishing good relationships between the Environment Agency and the central management for the industrial cluster would also be critical, since the approach will require continued cooperation from the industries in each cluster and a streamlined method of communication. Investment in terms of keeping an up-to-date, ‘whole site’ emissions inventory would facilitate continued, periodical modelling.

Communities living near these industrial clusters may also benefit from nowcasting or forecasting systems that integrate model and measurement data in order to predict air pollution levels and provide advice to minimise exposure of sensitive individuals.

Built environments

Urban and industrial built environments influence flow and dispersion processes. For example, buildings increase mechanical mixing and influence heat flux processes. While the influence of built environments on dispersion has been well documented in the literature, and there are numerous monitoring networks that have helped with the development of modelling tools, the impact of releasing emissions into built environments can be difficult to quantify. In some rural or segregated industrial locations, measuring the impact of the whole site is sufficient, so the built environment does not need to be considered. However, in urban and larger industrial areas, distinguishing the impact of a particular release from other sources can be difficult, due to non-linear interactions which complicate the Environment Agency’s ability to regulate effectively.

For most rural industry permit applications, only the process contribution is calculated, that is, it is not considered necessary to explicitly account for other sources in the vicinity (since their approximate contributions are typically accounted for in the background concentration). For pollutants strongly influenced by chemical processes, broad assumptions are made, for example, assuming that NO_2 is a fixed proportion of NO_X. However, in built environments, complex morphologies and overlapping plumes may influence dispersion processes and chemical processes, and these should be taken into account in any modelling study. This may be straightforward for some pollutants, but for others it is more complex because chemistry necessitates the modelling of total concentrations.

Modelling methods allow for the influence of the built environment on dispersion processes at a range of resolutions. Computational fluid dynamics (CFD) models represent flow and dispersion processes around buildings in detail. However, CFD has limitations in terms of explicitly calculating the required regulatory metrics, and accounting for some atmospheric stability and chemical processes (see section A4.5). Computational resources also limit CFD applications in urban areas, although the models are suitable for representing most industrial sites. Gaussian plume models parameterise the influence of buildings on flow and dispersion in several ways, which can lead to uncertainty associated with model predictions very close to buildings on an hour-by-hour basis. However, it is standard practice to use these models to calculate regulatory metrics that have no temporal dependence (means and percentile values), therefore reducing uncertainty associated with near-building modelling outputs. Coupled systems, for example, using CFD flow and turbulence fields within Gaussian plume dispersion models, may improve modelling of industrial sources in built environments.

The influence of the built environment on boundary layer flows is represented at larger scales within dispersion models via the surface roughness parameter. This parameter can either be estimated using broad categorisations relating to building density, or else explicitly calculated from three-dimensional (3D) digital representations of buildings, using a suitable algorithm (Macdonald and others, 1998; Di Sabatino and others, 2010). The influence of the built environment on heat flux processes may not be explicitly accounted for in models if measured meteorological data from a distant site are used as input. The urban heat island effect strongly influences heat exchanges in urban areas, which alters atmospheric stability and the structure of the boundary layer, impacting on dispersion processes.

Monitoring in built environments is regularly used as part of many air quality assessments, and many air quality assessments rely on long-term monitoring data within built environments. However, when monitoring in urban areas, it can be difficult to disaggregate the impact of a particular source from background pollution levels and other sources in the vicinity. Despite the above, there are methods, such as multivariate statistical analyses and Positive Matrix Factorisation (PMF) that can identify certain markers for apportioning contributions to sources, such as contributions from vehicles or woodburning. These methods are not, however, available with standard measurement methods (such as LCS or passive samplers), as standard methods do not afford the level of data required to perform these types of analyses. Such detailed source apportionment methods require the enrolment of complex monitoring equipment such as reference monitors or the installation of a supersite.

Where these source apportionment techniques are not suitable, it may be that emissions measurements, which commonly differ from permitted ambient levels, are important for quantifying the source impact; emissions measurements can be used as input to a model. Where emissions measurements are unavailable, it is advisable to model using worst-case emissions.

3. Main findings and options for future exploration

Main findings in terms of options for research in modelling, monitoring and integration methods are summarised in Table 5. The consultation process and literature review have identified several common themes, which have led to a series of options that would benefit the air quality assessment community; these are set out in Table 6.

Table 5: Main findings

Topic	Finding
Monitoring methods	There are a number of monitoring methods available which are suitable for a range of pollutants. The different methods offer varying temporal resolutions, spatial coverages and purchase costs. Each method is, however, associated with its own inherent uncertainty, and its application does, therefore, require careful consideration to ensure that the technique is fit for purpose. The rise in low-cost sensors (LCS) could potentially expand geographical coverage and enable access to monitoring equipment for the wider population. However, it has also highlighted the importance of equipment certification and the need for guidance to be followed when using any monitoring device.
Modelling methods	Models can potentially be developed to assess the impact of new activities and fuels. Models are available that can represent processes at small and large temporal and spatial scales. Joining one model with another, or with measurements, also allows a range of scales to be accounted for. Although underlying model formulations should be verified by model developers, the results of model applications are highly dependent on correct model configuration. Model users should be encouraged to compare results with measurements, and/or to provide explanations for model results.
Integrated monitoring and modelling methods	Measurements are commonly used as inputs to models, for calibration or as boundary conditions. In general, the more complex methods for integrating modelling and monitoring are not widely available for standard air quality assessments. However, some integration techniques (for example, data assimilation, machine learning (ML)) are well established in fields other than air quality. With the increasing availability of air quality measurement data sets, reviewing the applicability of these techniques to air quality applications may benefit the air quality practitioner community.

Table 6: Options for future exploration

Topic	Options for research
Guidance	There are existing modelling and monitoring guidance documents that have been generated for different groups, committees and users. Consolidating these documents with those written by the Environment Agency/Defra into a central place would streamline air quality assessments. The review has highlighted several areas, such as deposition modelling and low-cost sensors, where additional guidance could be beneficial to ensure they are applied correctly.
Protocols	A coordinated approach to air quality assessments of common, complex situations, such as industrial clusters, could be facilitated by establishing protocols, including preparing guidance and creating steering groups.
Monitoring networks	Extensions to the national monitoring networks, such as the National Ammonia Monitoring Network (NAMN), could assist with documenting concentrations in areas that are currently sparsely covered, including coastal areas. As additional monitoring devices are certified, there is also the potential to complement existing monitoring networks with alternative technologies, although this would depend on the requirements of the monitoring network. Investment in lower accuracy monitors to map the state of pollutants across large geographical areas could help with targeted placement of higher accuracy monitors.
Tool suitability	A comprehensive set of monitoring and modelling tools exists, but all tools have limitations, for instance in terms of their spatial and temporal applicability. The information presented in this study could be summarised to inform the air quality community about tool suitability for a range of common air quality assessments. It is important to keep such guidance updated to reflect current tool capabilities.
Database development	The Environment Agency, alongside other regulatory bodies, holds an extensive catalogue of monitoring data, which could be a valuable resource for the research community, particularly with respect to cumulative pollutant exposure and potential compliance issues. Establishing a secure and robust database, in collaboration with other bodies, and subsequently a relationship as a data provider, could be highly beneficial and an option to consider.
Inventories	To ensure that the modelling techniques used within air quality assessments are robust and defensible, periodic reviews into emissions databases, particularly with respect to new fuels and sources would be useful. Validating emissions inventories, including emissions measurements, could also help in quantifying impacts in complex environments.

4. Concluding remarks

This report has presented a number of monitoring, modelling and integration methods that are available to the Environment Agency for air quality assessments. In some cases, the methods are already applied in air quality assessments, while for others, additional research is required to realise the potential of the method. The air quality field is rapidly evolving, and therefore regular reviews of the identified methods may be necessary.

Three of the initially identified integrated modelling and monitoring methods encompass a range of approaches, specifically data assimilation, machine learning/deep learning (ML/DL) and inverse modelling. Of these, data assimilation and ML/DL are widely used for data analyses beyond the field of air quality. Consequently, there are many approaches that could be applied to air quality studies, and identifying the 'best' method for a particular situation may mean reviewing applications beyond air quality. Studies that compare and evaluate integration methods would be useful to air quality practitioners because they can help users to select appropriate methods and avoid incorrect applications. Appendix 3.4 outlines 2 examples of the kind of study that can help. Specifically, it outlines 2 ongoing Environment Agency studies of inverse modelling methods for estimating emissions. The studies include a broad review of inverse modelling and testing of methods for ease of use. They also compare the applicability and accuracy of different methods, including the collection of monitoring data. Such comparison and evaluation studies can inform the Environment Agency's development of a regulatory protocol for inverse modelling.

This project has progressed in parallel with a separate project on the drivers of future changes to air quality – a scoping study (SC220032/R) (Environment Agency, 2023a). While each project has been considered separately, the 2 projects are intrinsically linked. For example, changes in policy, behavioural shifts and the emergence of new technologies will dictate the future requirements for monitoring and modelling. Similarly, developments and results provided by monitoring and modelling techniques have the potential to shape future policy decisions and guide societal changes.

One such example may be the emergence of hydrogen as an alternative to fossil fuels. While beneficial from a carbon perspective, and therefore aligning with the government's Net Zero agenda, combustion of hydrogen leads to the production of NOx. In this context, current trends in monitoring data show that concentrations of NOx across England are generally reducing. However, if hydrogen-fuelled technologies become mainstream, monitoring data could demonstrate a reversal of the current trend, forcing policymakers to review NOx legislation.

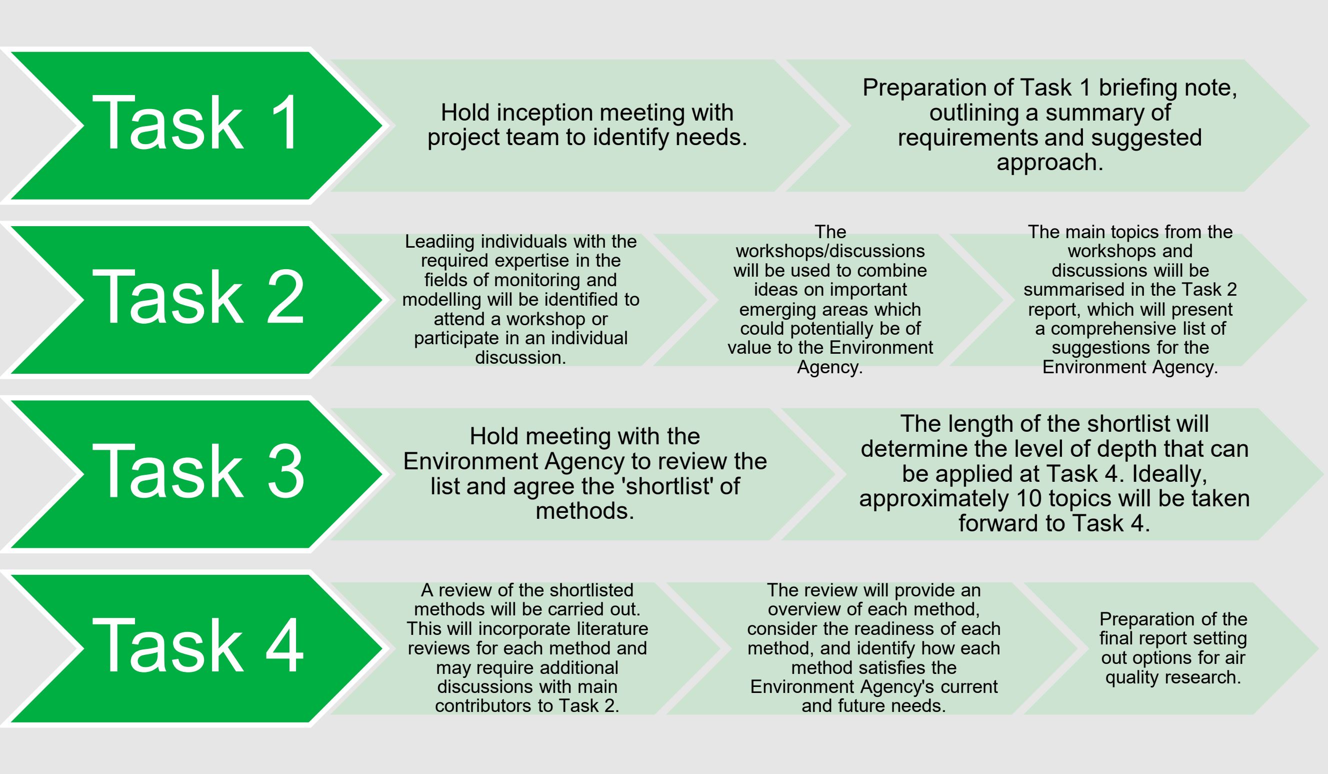
It would, therefore, be useful to consolidate the findings of the 2 projects and resolve the relationship between drivers and changes, and monitoring, modelling and integration techniques.

Appendix A1 Project approach

The project was divided into 4 main tasks:

- **Task 1** – gathering preliminary information on the Environment Agency’s assessment needs, based on an initial discussion with the Environment Agency.
- **Task 2** – synthesising information from leading experts in the field of air quality through a series of workshops and individual discussions to produce a comprehensive list of methods that may be of interest to the Environment Agency.
- **Task 3** – defining a shortlist of methods, based on a discussion of the comprehensive list with the Environment Agency project steering committee.
- **Task 4** – carrying out a high-level literature review of each shortlisted method, considering its usefulness and practical applications to the Environment Agency.

The actions undertaken as part of each project task are described in more detail below.



Task 1	Hold inception meeting with project team to identify needs.	Preparation of Task 1 briefing note, outlining a summary of requirements and suggested approach.	
Task 2	Leadiing individuals with the required expertise in the fields of monitoring and modelling will be identified to attend a workshop or participate in an individual discussion.	The workshops/discussions will be used to combine ideas on important emerging areas which could potentially be of value to the Environment Agency.	The main topics from the workshops and discussions wiill be summarised in the Task 2 report, which will present a comprehensive list of suggestions for the Environment Agency.
Task 3	Hold meeting with the Environment Agency to review the list and agree the 'shortlist' of methods.	The length of the shortlist will determine the level of depth that can be applied at Task 4. Ideally, approximately 10 topics will be taken forward to Task 4.	
Task 4	A review of the shortlisted methods will be carried out. This will incorporate literature reviews for each method and may require additional discussions with main contributors to Task 2.	The review will provide an overview of each method, consider the readiness of each method, and identify how each method satisfies the Environment Agency's current and future needs.	Preparation of the final report setting out options for air quality research.

A1.1 Task 2 Consultation approach

Purpose of the workshops and discussions

The purpose of the workshops and discussions was to synthesise information from leading individuals at the forefront of the monitoring and modelling fields relating to emerging areas of potential value to the Environment Agency. Prior to the workshops and discussions, each individual was provided with the following questions:

- Modelling and monitoring:

    - Do any techniques need more explanation to ensure that the method is ‘fit for purpose’?
    - Do any techniques need more guidance on how to apply the method?
    - Are there any ‘better’ methods for consideration?
- Integrating modelling and monitoring:
    - What are the current main methods integrating monitoring and modelling?
    - How could these methods be improved?
    - Are there any ‘better’ methods for consideration?
- Monitoring networks:
    - What are the main criteria when designing an air quality monitoring network?

The responses were subsequently discussed and interrogated further as part of the workshops and meetings. Two workshops and 5 additional discussions with individuals or organisations were carried out.

Attendees at workshops and discussions

Workshop 1, on Tuesday 14 February 2023, 2pm to 4.30pm, included contributions from the following individuals:

- Chris Dore (Aether), specialist in emissions inventories, monitoring and measurements.
- Roy Harrison (University of Birmingham), specialist in monitoring of particulate matter.
- Richard Maggs (Bureau Veritas), project manager for Defra’s Automatic Urban and Rural Network (AURN).
- David Carruthers (Cambridge Environmental Research Consultants (CERC)), specialist in modelling techniques.
- James Allan (University of Manchester), specialist in monitoring techniques.
- Nick Martin (National Physical Laboratory), specialist in monitoring methods, including low-cost sensors and ammonia measurements.

Workshop 2, on Wednesday 15 February 2023, 9:30am to 12.00pm, included contributions from the following individuals:

- Steve Moorcroft (Air Quality Consultants (AQC)), specialist in modelling and monitoring approaches.
- Huw Woodward (Imperial College London), specialist in computational fluid dynamics (CFD) modelling.
- Amy Stidworthy (CERC), specialist in modelling techniques, including inverse modelling.
- Chris Connor (Scottish Environment Protection Agency (SEPA)), specialist in regulatory requirements.

An additional meeting was held with Brian Kerridge from Rutherford Appleton Laboratory (RAL), including 3 researchers associated with the Remote Sensing Group (Barry Latter, Gareth Thomas and Ka Lok Chan). These discussions focused on the opportunities afforded by remote sensing and satellite measurements.

A further meeting was held with Massimo Vieno and Eiko Nemitz from the UK Centre for Ecology & Hydrology (UKCEH), which focused on the applications of long-range transport models and the potential role of ammonia in future air quality management.

The authors also held a meeting with Tom Gardiner from the National Physical Laboratory to discuss the applications of ground-based remote sensing technology and to discuss the limitations to the technique with respect to air quality assessments.

Individual discussions were also carried out with Roger Timmis and Rob Kinnersley from the Environment Agency, to understand the Environment Agency's regulatory requirements and additional consultee duties.

A1.2 Task 2 Air quality assessment methods review approach

Following the workshops and individual discussions, the main themes, methods and emerging areas were grouped according to their application.

The modelling methods outlined in Table A2.1 in Appendix A2 encompass a range of different modelling approaches, as well as specific model features that address particular release types.

The monitoring methods outlined in Table A2.1 in Appendix A2 encompass a range of types, resource requirements and network size. The selected methods also consider the importance of geographical coverage.

The workshops and meetings also identified a range of methods that can be used to integrate modelling and monitoring data; these methods are summarised in Table A2.1 in Appendix A2.

Characterisation of air quality methods

For each method in Table A2.1 in Appendix A2, the following information is provided:

- method name
- brief description and issue or application
- relevance to the project, in terms of monitoring, modelling or integration
- spatial scale, where:
    - **H** = high spatial resolution (for example, centimetres/metres)
    - **M** = medium spatial resolution (10s to 100s of metres)
    - **L** = low spatial resolution (kilometres and greater)

    - In some instances, defining a spatial scale is not appropriate, indicated by 'N/A'

- Temporal scale, where:
    - **H** = high temporal resolution (sub hour frequency)
    - **M** = medium temporal resolution (hourly frequency)
    - **L** = low temporal resolution (daily/annually)

The summary of the characterisation is presented in Table A2.1 in Appendix A2.

A1.3 Additional topics identified in Task 3

Following the meeting with the Environment Agency project steering committee during which the list of methods was discussed, the following topics of interest were also introduced for consideration as part of Task 4:

- assessment of amines arising from carbon capture, utilisation and storage (CCUS)
- modelling of intensive farming activities
- validation of air quality modelling in complex coastal and terrain scenarios
- cumulative pollutant exposure
- noise monitoring[1]

A1.4 Methods excluded from further discussion in Task 3

Following discussions with the Environment Agency project steering committee, a number of methods identified during the workshops and discussions were not progressed; these are presented in italics in Table A2.1 in Appendix A2. Methods were not progressed because either they are:

- subject to a separate workstream
- not considered to be of sufficient use to the Environment Agency in the context of air quality assessments

A brief explanation of each excluded method is provided in Appendix A3.

---

[1] It is understood that there are 3 ongoing Defra-funded projects, covering gaps in the Environment Agency's current repertoire, therefore, noise is outside of the scope of this project and covered separately elsewhere.

Appendix A2 Comprehensive list of air quality methods

Table A2.1: Comprehensive list of methods [a]

Item	Method	Brief description and issue or application	Project area	Spatial scale	Temporal scale
1	Gaussian plume modelling	Widely used across the air quality community to model concentrations at discrete receptors, with dispersion parameters dependent on distance from source, meteorological data and emission parameters.	Modelling	**L – H**	**L – M**
2	Lagrangian Gaussian puff modelling	Releases are modelled as a series of puffs, allowing variable emissions and release properties with time.	Modelling	**L – H**	**L – H**
3	Lagrangian particle modelling	Statistical model of turbulent diffusion, based on the position of a particle at a given moment in time relative to its initial location.	Modelling	**L – H**	**L – H**
4	Grid-based Euler models	Complex multiphase model often used for modelling long-term chemical transport. Involves solving a series of momentum and continuity equations.	Modelling	**L**	**L – M**
5	Computational fluid dynamics (CFD) modelling	CFD typically involves the calculation of fluid (air) flow and heat fluxes for applications where buildings, terrain and other structures strongly influence flows. CFD models commonly include air pollutant dispersion modules.	Modelling	**H**	Commonly a set of isolated meteorological conditions corresponding to distinct wind sectors.

6	Modelling of non-linear processes: complex chemistry/ radioactivity	Chemical and radioactive decay processes are non-linear. Atmospheric chemical reactions can strongly influence ar quality concentrations. Includes amine chemistry. Deposition and resuspension processes can be non-linear (notably semi volatiles such as ammonia and organic aerosols). Resuspension in this context is when a pollutant deposited on a surface is re-released into the atmosphere, by evaporation in the case of ammonia or wind-blown dust for particulate matter (PM). It is non-linear because it is a ‘competition’ between the deposition and resuspension drivers.	Modelling	**L – H**	**M**
7	Dry and wet deposition modelling	Pollutants deposit at the ground through dry and wet deposition processes. In-plume concentrations reduce as a result of deposition.	Modelling	**L – H**	**L – M**
8	Complex terrain wind field modelling	The influence of complex terrain (for example, hilly, mountainous, forested and coastal areas) on dispersion must be accounted for, where relevant.	Modelling	**L – H**	**L – M**
9	Nested/ coupled modelling systems	Systems consisting of more than one model. Can be one-way coupling, or models can link dynamically (feedback). Suitable for studies where a range of spatial or temporal scales and resolutions is important.	Modelling	**L – H**	**L – H**
10	Ensemble modelling	Modelled concentrations are derived from multiple model results in order to scope uncertainties.	Modelling	**L – H** depending on model(s) considered	**L – H** depending on model(s) considered

-	*Odour modelling*	*Odour is modelled as a non-reactive air pollutant release.*	*Modelling*	***M – H***	***L – H***
-	*Dense gas release modelling*	*Negatively buoyant plumes are a subset of all atmospheric pollutant releases.* *Dense gas releases can be particularly hazardous in terms of environmental health.*	*Modelling*	***H***	***M – H***
-	*Wind tunnel modelling*	*Physical simulations of pollutant dispersion within a wind tunnel.*	*Modelling*	***H***	*Commonly a set of isolated meteorological conditions corresponding to distinct wind conditions.*
11	Passive samplers	Small plastic tubes that contain a filter onto which pollutants of interest are absorbed. Advances in technology mean that accuracy of reference-equivalent instruments can be replicated at much lower cost.	Monitoring	Dictated by the number of samplers.	**L**
12	Low-cost sensors	Sensors designed to provide indicative measurements of regulated pollutants in ambient air, available at lower cost than reference-equivalent instruments.	Monitoring	Dictated by the number of sensors.	**M – H**
13	Reference monitors	Instruments that align with the measurement methods specified in the European Union (EU) Directives.	Monitoring	Dictated by the number of monitors.	**M – H**
14	Urban supersites	Large research stations comprising state-of-the-art technology to probe the atmosphere in greater	Monitoring	N/A	**M – H**

		detail than reference monitors. Measurements are split into 3 main groups: gases (for example, ozone, NO_2, ammonia, methane), aerosols (for example, PM, black/brown carbon, particle size and number), and meteorology (for example, wind speed, precipitation rate, temperature, boundary layer height, solar radiation).			
15	Mobile air quality monitoring	Mounting monitoring equipment on ground vehicles (for example, vans), aerial vehicles (for example, drones) or aircraft.	Monitoring	Depends on technique – can move around, but measurement limited to that area (vans). Drones/planes can cover larger areas.	**M – H**
16	Ground-based remote sensing measurements	Ground-based remote sensing equipment can measure the spatial distribution of concentrations within a plume and the movements of plumes of particles and gases.	Monitoring	**M – H**	**M – H**
17	Siting of monitors and network optimisation	Decision-making process for locations of monitors and their use to build up a network.	Monitoring	**L – H** (depends on purpose of network).	**L – H** (depends on monitoring technique used).
18	Hierarchical networks	A coordinated network with a large number of lower accuracy monitors connected to a smaller number of higher accuracy monitoring equipment.	Monitoring	Dictated by the number of monitors.	**M – H**: Would vary depending on monitoring technique.

19	Data assimilation	Combining model and monitoring data to calibrate models and interpolate between measurements.	Integration	**L – H**	**L – H**
20	Machine learning (ML)/ deep learning	Applying ML algorithms to air quality. Air quality models built based on sample training data set to predict air quality.	Integration	N/A	**L – H**
21	Satellite measurements	Indicative pollutant concentrations derived from satellite imagery.	Integration	**L** – can have gaps in data (cloud).	Non-continuous snapshots.
-	*Receptor modelling*	*Identification/quantification of source types of pollutants contributing to air quality at a defined receptor location.*	*Integration*	*N/A – composition based*	***M – H***
-	*Inverse modelling for emissions estimation*	*Uses monitoring data to determine the source emissions.*	*Integration*	***M – H***	***L – H***

[a] Items in italics indicate methods that, following completion of the list, were not researched further following discussions with the Environment Agency.

Appendix A3 Methods not progressed following discussion with the Environment Agency

Following the meeting with the Environment Agency project steering committee during which the list of methods was discussed, several methods and applications were withdrawn from further consideration. A brief overview of each method or application is provided below.

A3.1 Odour modelling

Odour modelling was not explicitly discussed in the workshops or meetings, but the 2021 Atmospheric Dispersion Modelling Liaison Committee (ADMLC) report ‘A Review of Approaches to Dispersion Modelling of Odour Emissions and Intercomparison of Models and Odour Nuisance Assessment Criteria’ (Price and others, 2021) is very relevant to this topic. The ADMLC report:

- summarises main concepts in odour criteria and assessment
- reviews odour criteria and methodologies in different countries
- reviews the range of models used for odour assessment
- summarises selected odour modelling validation studies
- presents a model inter-comparison (Gaussian plume and Lagrangian models)
- discusses the efficacy of the different approaches to odour dispersion modelling

A3.2 Dense gas release modelling

Dense gas modelling was not explicitly discussed in the workshops or meetings, but the 2021 ADMLC report ‘Review of dense-gas dispersion for industrial regulation and emergency preparedness and response’ (Health and Safety Executive, 2021) is very relevant to this topic. The ADMLC report:

- summarises 69 dense gas incidents
- reviews 64 dispersion models
- summarises 63 dense gas dispersion experiments (fields trials/wind tunnel studies)
- discusses future trends and emerging technologies

A3.3 Wind tunnel physical modelling

Wind tunnel modelling involves physical simulations of pollutant dispersion within an aerodynamic tunnel. Atmospheric wind tunnels are available in Research Council and academic locations (such as the National Environment Research Council (NERC) National Centre for Atmospheric Science (NCAS) Environmental Flow (EnFlo) facility hosted by the

University of Surrey) and commercial locations (such as RWDI and BRE). Additionally, University College London is developing the ‘Controlled Active Ventilation Environment’ (CAVE) facility, which is a life-sized, enclosed environment that can be used to take climate and air quality measurements corresponding to a wide range of situations (University College London, 2023).

Qualitative wind tunnel assessments can be used to visualise flow and dispersion of pollutants, and concentrations can be determined using high sensitivity methods. When used to determine concentrations, wind tunnel modelling is commonly used alongside computational fluid dynamics (CFD).

Flow and concentration data from wind tunnel studies can be used to parameterise dispersion models. However, wind tunnel data sets are limited in terms of the range of meteorological conditions considered, in part because it is difficult to achieve a statistically steady boundary layer of sufficient thickness within the length of the wind tunnel, but also because physical modelling is very resource intensive. Usually only a subset of real world atmospheric meteorological conditions is modelled, for instance neutral and stable conditions, for a subset of wind speeds. The EnFlo facility can simulate thermal stratification, which increases capability in terms of the meteorological conditions that can be represented. Scaling is required in order to convert between wind tunnel dimensions (length and concentration) to real-world situations (Kozmar, 2010).

Due to the subset of conditions considered, the outputs from wind tunnel modelling do not enable direct comparisons with environmental standards, and processing is necessary to generate long-term equivalent concentrations. Also, there are significant resource limitations in terms of gaining access to wind tunnel modelling facilities and the associated expertise required to perform experiments. Therefore, they are not suited for compliance-type assessments, but better for identifying constraints and/or developing model parametrisations.

There may be a requirement for additional specialist guidance to enable the correct interpretation (some expertise is already available in-house), and the Environment Agency would need to outsource wind tunnel work as it requires specialist facilities.

A3.4 Inverse modelling for emissions estimation

There are currently 2 ongoing Environment Agency projects into the applications of inverse modelling for estimating emissions (Environment Agency, 2023b).

The first project includes a review of the different methods that can be used to quantify emissions from the whole site, or from sources separately within a site.

Whole site methods include:

- horizontal plume transects with 1D Gaussian profile fitting
- 2D vertical plane measurements with bi-Gaussian fitting
- airborne mass balance

- tracer dispersion method
- stationary plume transect from single location measurements
- eddy covariance
- Gaussian plume modelling with direct search

Within site methods include:

- high-resolution spatial survey monitoring
- backward Lagrangian stochastic approaches
- semi-analytical Gaussian plume inversion
- Bayesian inversion frameworks
- Gaussian plume dispersion with genetic algorithms
- adjoint modelling in complex flow fields
- machine learning (ML)

For some methods, the quality of monitoring data impacts on the reliability of modelled emissions, although measurement uncertainty may be accounted for within some methodologies.

The first project also includes a summary in terms of applicability and testing 3 methods (simple Gaussian fitting, backwards Lagrangian stochastic and Bayesian inversion) at 3 generic landfill sites emitting methane.

The second project involves applying Bayesian inversion techniques incorporating a commercially available Gaussian model to estimate methane emissions at a single site, focusing on the analysis of temporal variations.

A3.5 Receptor modelling

Receptor modelling requires multivariate statistical analysis methods such as Positive Matrix Factorisation (PMF) to carry out analysis of detailed atmospheric composition measurements, which are available from, for example, chemical mass balance (CMB) measurements, Aerosol Chemical Speciation Monitor (ACSM) measurements or X-ray fluorescence analysis. The evaluation of secondary material (for example, secondary organic aerosol) is currently dependent on these models and deterministic methods. PMF can also be used to carry out analysis of contributing sources to different size and composition fractions of particulate matter. Most commonly, published modelling based on PMF is determined using the US EPA software US EPA-PMF 5 (United States Environmental Protection Agency, 2023). However, while it is user-friendly, this tool is no longer being supported or developed by the US EPA. Preceding this is the PMF version 2 (PMF2) algorithm, a Fortran executable, which remains widely used for source apportionment studies (Paatero, 1997). The program IGOR (Interface for Geospatial Operations Research) provides an interface for running the PMF2 model, allowing for data preparation and diagnostics of performance. It is freely available (for academic use) and is maintained by Colorado University (Ulbrich and others, 2009). There is also an open-source module in R (pmf-tools) which runs the PMF2 executable that can resolve source profiles, contributions and uncertainty (Takahama, 2015). Nonetheless, as in the case of the US EPA software, poor understanding of the software and methodology gives potential for misuse, particularly since the EPA no longer provides troubleshooting advice. Further, long-term multicomponent aerosol data on a daily timescale is needed; otherwise, the model can be unstable.

FAIRMODE CT1 activity includes a guide for source apportionment with receptor models (Clappier and others, 2022) which can be accessed openly, and which seeks to support air quality management processes.

Appendix A4 Specific methods

The following sections focus on demonstrated, or potential, use of a variety of monitoring, modelling and integration approaches for air quality assessments. However, identifying that a particular method is suitable for air quality assessment is only the first step in ensuring that a particular method will generate defensible data sets suitable for regulatory applications. The following items help to ensure that models and measurement equipment are applied correctly:

- **User documentation** for example, user guides, technical specifications
- **Training and support**
  - This can be in the form of organised training courses or informal support from more experience colleagues
- **Guidance**
  - This is required in order to ensure that the applications are 'fit-for purpose' and can include:
    - step-by-step instructions
    - example case studies
    - signposting to required data sets (for example, inputs for models)

A high-level summary of the shortlist of topics is provided below.

A4.1 Gaussian plume modelling

Gaussian plume modelling is a common physics-based approach to assessing the impact of a wide range of pollution sources (point, line, area, volume, road, grid). Gaussian plume models are well established, practical to use and have relatively limited resource (human and computational) requirements. They are, therefore, routinely used for air quality assessments. There are a number of models available, including Atmospheric Dispersion Modelling System (ADMS) (Carruthers and others, 1994), American Meteorological Society and United States Environmental Protection Agency Regulatory Model (AERMOD) (Cimorelli and others, 2005) and the Danish 'Operationelle Meteorologiske Luftkvalitetsmodeller' (OML) (Berkowicz and others, 1986). Atmospheric stability is commonly categorised using a Monin-Obukov length stability parameter, which allows modelling at hourly resolution (consistent with most meteorological data records). Features vary hugely between models, with most suitable only for dispersion of point sources over flat uniform terrain. Many models include plume ruse and wet and dry deposition, while a very few include more advanced features such as:

- plume chemistry (NO_X, SO_X and amine)
- odour releases; fluctuations
- coastline and marine boundary layer effects
- flow and dispersion around buildings

- urban morphology, including effect of street canyons, tunnels and elevated roads

Does the method need more explanation or guidance to ensure it is 'fit for purpose'?

Widely used ‘off-the-shelf’ Gaussian plume models such as ADMS and AERMOD have openly available user guides, technical specifications and model evaluation documentation. These resources provide information on how to configure the model, and how to make use of particular model features. Software support and training is also available, which facilitates application by non-experts. Cambridge Environmental Research Consultants (CERC) operates an ADMS helpdesk service, so that model users can ask questions about their particular model application. As part of its support package, CERC runs ADMS user group meetings annually, which generate case studies.

Limitations

Most Gaussian plume models use homogeneous meteorology to drive dispersion, which limits the spatial range of applicability to around 50km, depending on the model domain. Gaussian plume models are ‘steady state’, meaning that a new solution is calculated for each successive (usually hourly) set of meteorological data. This leads to inaccuracies, particularly in their treatment of low wind conditions. Gaussian models are not able to model all processes in detail, instead relying on parameterisations and simplifications where more complex effects are included in the models (for example, close to buildings). This ensures that they are practical to use but can increase uncertainties. Within a particular model, there are some limitations in the combination of model features that may be used together; for example, dispersion from line and area sources is not able to take account of the buildings-affected flow fields calculated in either ADMS or AERMOD. These limitations arise both from scientific and computational complexities, and resource constraints.

Possible improvements

Gaussian models that are developed for community use such as ADMS and AERMOD undergo continual development, including inclusion of new features. These features can reflect new requirements (for example, the need to model amine chemistry processes in relation to CCUS) and new understanding (for example, improvements to dispersion processes in the vicinity of buildings through the study of wind tunnel and CFD modelling results).

The relative simplicity of Gaussian models lends itself well to inclusion within dynamic/ comprehensive systems such as the Air Pollution Assessment Service (APAS) (under development by the Joint Nature Conservation Committee (JNCC)), and scenario modelling. Improved coupling of Gaussian models to systems that account for processes at different spatial scales is beginning to allow wider applications, for example:

- coupling to regional modelling systems (mesoscale meteorological models and CTMs)
- coupling to microscale emissions and flow (CFD) models

A4.2 Lagrangian Gaussian puff modelling

Lagrangian Gaussian puff modelling is a non-steady state method considering a full range of temporal and spatial scales. The method takes into account spatially and temporally varying meteorology (for example, from mesoscale meteorological models such as weather research and forecasting (WRF)) to allow puff dispersion over long time periods (more than a day) and large distances (100s of km). The spatial extent of each puff is defined using a Gaussian formulation, similar to a Gaussian plume in the vertical and crosswind directions, but includes along-wind Gaussian growth and decay. Puffs may be buoyant, passive or dense.

Puff modelling commonly requires more resources to run in comparison to a Gaussian plume model. Therefore, puff modelling should only be considered as an option for a particular application when limitations of the Gaussian plume model (steady state with homogeneous meteorology) may make plume modelling unsuitable. These can be broadly categorised as:

- long timescale – puff models can account for changing meteorology and chemical reactions over long (>1 hour) timescales, and mesoscale changes in flow
- very short timescale – pull models can represent releases that occur at timescales less than an hour, for example, corresponding to emergency releases

The most widely used puff model is CALPUFF (California Puff) (Scire and others, 1990), currently developed by Exponent (CALPUFF Modeling System, 2023). The CALPUFF model comprises CALMET (Scire and others, 2000), CALPUFF and CALPOST for meteorological, dispersion and post-processing calculations respectively. SCICHEM (Chowdhury and others, 2015) is a puff model that incorporates complex gas, aqueous and aerosol phase chemistry processes. It is maintained by Ramboll and has been developed from the US Government SCIPUFF (Second-order Closure Integrated Puff) (Sykes and others, 1993) model. Other puff models include CERC’s ADMS-STAR (2023), which calculates instantaneous air concentrations, and accumulated wet and dry deposition, for radiological or chemical emissions, and ADMS-PUFF (2023) which models dense gas releases.

Does the method need more explanation or guidance to ensure it is 'fit for purpose'?

All the puff models mentioned in the previous section have openly available user guides and technical specifications. These resources provide information on how to configure the model, and how to make use of particular model features. Software support and training is also available, which facilitates application by non-experts.

In terms of case studies, there are relatively few examples of UK applications of CALPUFF, although it is widely used in Canada and elsewhere. CALPUFF ceased to be a US regulatory model in 2017. There do not appear to be many applications of SCICHEM in the literature, which may be related to the relatively large computational overhead associated with the complex chemistry calculations. ADMS-PUFF and ADMS-STAR have specialist users.

Limitations

Puff models require larger computational resources, in terms of both meteorological and dispersion calculations, in comparison to plume models. They also require more human resource time to configure. Therefore, their use is only warranted for the cases where plume models are unsuitable (highlighted above).

Possible improvements

Computational resources would improve accessibility to puff models.

A4.3 Lagrangian particle modelling

Lagrangian particle dispersion models (LPDMs) are based on calculations following a random walk process through the atmosphere for a large number of particles (infinitesimally small air parcels). Concentration statistics (for example, mean or variance) are derived from the particle density, so sufficient particles need to be released to ensure the distributions of particles are ‘stable’. LPDMs are unsteady, these particles follow local flows, defined by the temporally and spatially varying meteorology, while the random component simulates the effects of turbulence. LPDMs are capable of simulating particle dispersion both forwards and backwards in time. They can model flow around buildings, complex terrain and coastal variations. LPDMs can also cover spatial scales from “dozens of metres” to global and are suitable for a range of wind-speeds and stability conditions (Pisso and others, 2019).

Unlike Gaussian plume models, LPDMs do not require assumptions about the shape of the concentration distribution. However, LPDMs are more computationally expensive than other dispersion models, such as Gaussian plume, especially for large-scale simulations, high concentrations, or to achieve results with a high level of statistical confidence. LPDMs should be used when conditions are unsuitable for computationally cheaper models or if backwards simulation or more detailed output data are required. Examples include where local flow is very complex (for example, in built environments, deep valleys, low wind speed conditions) and for larger mesoscale scales flows.

There are several commonly used LPDMs, including NAME, AUSTAL, FLEXPART, GRAL and HYSPLIT. NAME (Nuclear Accident ModEl) is the Met Office model, using meteorological data from their Unified Model and the ECMWF numerical weather prediction model. It is combined with a Eulerian model and is intended for medium distance to global ranges (Jones and others, 2007). Notably, NAME includes an air focused chemistry scheme using the Met Office global chemistry model STOCHEM (Collins and others, 1997). FLEXPART (FLEXible PARTicle) dispersion model is one of the most widely used, with a global user base (Pisso and others, 2019). FLEXPART was developed between 2 European universities (Universität für Bodenkultur (BOKU), Technische Universität München (TUM)) and the Norwegian Institute for Air Research. The AUSTAL model is the regulatory air dispersion (Ausbreitungsrechnungen nach TA Luft) model in Germany, developed for the German Environment Agency (Janicke and Janicke, 2002). FLEXPART and AUSTAL are capable of simulating first-order chemical reactions. The GRAL (Graz Lagrangian) model was developed by the iTnA at Graz University of Technology (Oettl, 2016). This model is an option for low-wind speed conditions. GRAL has an integrated micro-scale flow-field model which includes building effects. However, it has no chemistry capabilities. HYSPLIT (Hybrid Single-Particle Lagrangian Integrated Trajectory) model was developed by the National Oceanic and Atmospheric Administration (NOAA). It uses meteorological data from the North American Meso weather model to calculate advection and dispersion of the particles (Draxler and Hess, 1997). It is applied at large spatial scales, for example, modelling the global movement of radioactive isotopes (Bowyer and others, 2013). Chemistry modules may optionally be incorporated into HYSPLIT modelling.

Each model is widely cited in literature. However, there were relatively few examples of UK applications. The regulatory model, AUSTAL is widely used in Germany.

Does the method need more explanation or guidance to ensure it is 'fit for purpose'?

All the LPDMs described in the previous section are free to download, although some have commercially available packages. HYSPLIT provides a user forum, and in 2022 held a 4-day workshop. GRAL currently only provides tutorial videos online. The remaining LPDMs provide freely available user guides. AUSTAL also has a viewable ticket system for user issues. Excluding HYSPLIT, there were no user forums or upcoming training sessions (since 2019).

Limitations

As with all models, LPDMs have the potential to generate misleading results when configured incorrectly, and it is important to perform sensitivity testing to ensure defensible concentration predictions. For example, the final location of a particle trajectory differs depending on the sampling time of the meteorological data, resulting from the interpolation of the input wind fields (Bowman and others, 2013).

LPDMs require good quality meteorological data sets as input. These can be relatively computationally expensive to generate (for example, computational fluid dynamics (CFD), mesoscale meteorological models). LPDMs require substantial computational resources to model the many particles required to give sufficiently aggregated results to reduce statistical errors. The majority of LPDM packages account for limited chemical reactions, although NAME includes complex chemistry. Some allow for the addition of chemistry modules or work in combination with additional models. LPDMs have difficulty dealing with bulk effects, such as plume rise, and modelling of inhomogeneous flows may lead to issues such as particles collecting.

Possible improvements

Increased availability of computational resources and detailed atmospheric environment data would improve accessibility to LPDMs. Chemistry schemes in some models could be improved.

A4.4 Grid-based Euler models

Eulerian methods discretise a 3D geographical domain into boxes of fixed and/or varying dimensions and calculate the atmospheric composition at the centre of each box. In contrast, Lagrangian schemes follow air parcels, or volumes, and all the changes are calculated within the moving parcel of air. There are advantages and disadvantages to both approaches which are not discussed here. The majority of modern atmospheric chemistry transport models (ACTMs) have opted for a grid-based Eulerian approach to calculate the transport, chemical transformation and deposition processes which occur over a large range of temporal and spatial scales. ACTMs typically use numerical prediction models to provide the spatially and temporally varying meteorological data.

Many countries and organisations worldwide adopted these types of models for regional and national scale air quality assessment. The models generate 3D values of hourly to annual average air pollutant concentrations for a comprehensive range of pollutants. The chemistry is typically the most computationally expensive part of these models. Commonly, ACTMs use simplified chemistry schemes derived from, or evaluated against, the Master Chemical Mechanism (MCM). ACTMs are relatively complex to configure (and very complex beyond the ‘standard’ setup), and require moderate to high computing resources, commonly run in Linux environments. They often require high-performance computers, with a heavily parallelised code using the Message Passing Interface (MPI). These models are computationally expensive and use a compromised approach in order to ensure the most accurate representation of long-range pollutant transport. This is achieved by using a series of nested grids with increasingly fine resolution which are often set up for both the mesoscale meteorological model and CTMs. For example, modelling a region such as England could require a 27km x 27km grid for Europe, a 9km x 9km grid over the British Isles and a 3km x 3km grid over England.

A selection of commonly used Eulerian grid models are summarised in Table A4.1, which gives model name; a list of supported/compatible meteorological model(s); core model developers; and a main scientific reference. The majority of these models are developed through government-funded research, regulatory and/or meteorological organisations, apart from CAMx, which has developed commercially under contracts from local government and other organisations.

Table A4.1: Overview of widely used Eulerian grid CTMs

CTM	Supported meteorological model(s)	Core model developers	Reference
Community Modelling Air Quality (CMAQ)	WRF	US EPA	(Byun and Schere, 2006)
WRF-Chem	WRF	US NOAA	(Grell and others, 2005)
CAMx	WRF, MM5, RAMS	Ramboll	(Ramboll, 2020)
EMEP	WRF, ECMWF IFS	Norwegian Meteorological Institute and Chalmers University, Gothenburg	(Simpson and others, 2012)
CHIMERE	WRF, ECMWF IFS	IPSL/LMD	(Menut and others, 2021)
AQUM	Met Office Unified Model	UK Met Office	(Walters and others, 2019)
LOTOS-EUROS	WRF	US EPA	(Manders and others, 2017)
GEOS-Chem	Varies/WRF	Harvard University	(GEOS-Chem, 2023)

Does the method need more explanation or guidance to ensure it is 'fit for purpose'?

These models have associated user documentation, although in most cases this is written for experts. Some models include choices of modules for similar purposes, for example, different aerosol chemistry methods. Model users may have to review the literature and/or perform sensitivity testing in order to understand the differences between modules. Training courses are available for some models and user support is often provided through online forums (CMAQ, WRF-Chem) and/or user mailing lists (WRF-Chem, CHIMERE). Most of the models are now available on GitHub.

Limitations

The models can be applied at grid resolution of 1km, but at finer scales some of the parameterisations break down, for example, turbulence within the mesoscale model. Therefore, CTMs are suitable for modelling rural, suburban and urban background concentrations, but not at roadside.

As these models are relatively complex to configure and require significant resources to run, they are usually applied by experts. By virtue of the models accounting for multiple, complex processes, it can be difficult/time-consuming to investigate and explain model performance. It is also very difficult to assess the uncertainty of the complex systems.

Possible improvements

Coupling of regional models to finer resolution models such as Gaussian models allows systems to be developed that are able to model at a wider range of scales, for example, including roadside.

A4.5 Computational fluid dynamics modelling (CFD)

CFD is the technique of numerically solving the equations governing conservation of mass, momentum, heat and mass transfer to calculate fluid flow. Commonly, CFD models include equations that account for pollutant transport, therefore allowing air pollutant concentration calculations to be performed.

Only 3D CFD is useful for ambient air quality modelling. The models range in their level of complexity and, therefore, required computational resource (listed in order of increasing resource requirement):

- Reynolds-averaged Navier-Stokes (RANS) is a method whereby the mean flow is modelled, and turbulent eddies are parameterised (for example, k-epsilon (Yusuf and others, 2020)). The resulting flow field is either steady-state or captures only larger scale, periodic fluctuations.
- Large eddy simulation (LES) is an unsteady method, where the variations of large-scale turbulence are modelled over time; smaller-scale eddies are parameterised.
- Direct numerical simulation (DNS) involves the unsteady simulation of all turbulent length scales.

RANS has the fewest computational requirements, although resources are still significantly larger than running fully parameterised systems such as Gaussian plume models. It is likely RANS would be the most common type of CFD used directly for air quality assessments, in comparison to LES and DNS. However, LES may be suitable for accidental release modelling, where short-term variations in the source parameters are important and/or releases may be sufficiently large to influence local flow. LES approaches are also sometimes nested within mesoscale meteorological model outputs, to represent finer scale atmospheric motions. CFD model domains and computational grid resolutions relate to the dimensions of the physical and flow structures being modelled. Numerical stability limits for the underlying flow calculations require smaller model time-steps for finer grid resolutions. This causes a non-linear increase in computational expense with reducing grid size. Examples of commonly used CFD RANS models include OPENFoam (2023), Ansys Fluent (2023) and STAR-CCM+ (Siemens, 2023).

CFD models are commonly used in wind microclimate studies for assessing pedestrian comfort and safety, but the application of CFD to air quality modelling is less well established. CFD can be used to assess the near field influence of buildings and other obstacles on flow and, therefore, dispersion, with the potential to be useful for modelling releases in urban environments. CFD domain extents can be up to 10km or so, with output at metre resolution.

CFD model outputs have the potential to be used for other applications:

- to generate datasets that can be used to develop parameterisations within less computationally intensive models, for example, building modules within Gaussian plume models
- to optimise monitor placement

Does the method need more explanation or guidance to ensure it is 'fit for purpose'?

Expertise is required to run CFD models. For example, care is required to ensure that solutions are independent of the calculation grid definition and fully converged. High-resolution outputs give the illusion of accuracy, and it is important that modelled flows and concentrations are correctly interpreted.

Two COST (European Cooperation in Science and Technology) actions have generated guidance documents that provide some information on the application of CFD models, including air quality applications:

- COST Action 732: CFD Simulation of Flows in the Urban Environment (Franke and others, 2007)
- COST Action ES1006: Atmospheric Dispersion Models in Emergency Response Tools at local scale in case of hazmat releases into the air (European Cooperation in Science and Technology, 2015)

Microscale model application in the context of the European Air Quality Directive (The European Parliament and the Council of the European Union, 2008) is the topic of FAIRMODE’s WG4 (European Commission Joint Research Centre, 2023). There has been some discussion of approaches for re-combining subsets of CFD model outputs into annual metrics within this working group. The CFD modelling community would benefit from some guidance.

Limitations

The relatively large computational resource overhead associated with CFD means that the models are usually run for a subset of wind speeds/sectors, in other words, not for all hours within a year. Therefore, CFD models may be used to identify pollution hotspots and inform environmental planning. Typical modelled air pollutant concentration fields correspond to neutral meteorological conditions, for a single wind speed, for a range of wind directions (for example, 18 wind directions, every 20°). For neutral conditions, wind speeds can be scaled to represent a range of wind speeds, but:

- the relationship between wind speed and pollutant dispersion can be non-linear (inverse), so air pollutant dispersion calculations should be repeated for different wind speeds (rather than scaled)
- pollutant dispersion is dependent on atmospheric stabilities. CFD rarely distinguishes between neutral, stable and convective conditions, which is a limitation because stable/convective conditions lead to higher ground level impacts for ground-level/elevated sources compared to neutral conditions

The limitation of only modelling a subset of meteorological conditions makes it difficult to use CFD to calculate air quality metrics that require modelled concentrations for every hour of the year (for example, annual averages and threshold exceedances).

As for many steady-state models, the RANS algorithms break down at low wind speeds, which limits their application in stagnation conditions.

CFD models rarely account for chemistry processes in any detail, so additional modelling/post-processing is required for pollutants strongly influenced by short-spatial scale chemical reactions, for example, NO_2.

Possible Improvements

With increased computational resource going forward, CFD models may be applied more comprehensively, for instance over larger domains, with better support for a range of meteorological conditions and other increased capabilities.

One method of overcoming some of the limitations associated with air pollutant dispersion modelling within CFD is to use the flow field output from CFD models to drive dispersion within Gaussian plume and particle models. This approach allows modelling of near-field atmospheric chemistry and some consideration of atmospheric stability. An option to use CFD flow fields within ADMS is available, although examples of its use are limited. The Chartered Institution of Building Services Engineers’ (CIBSE) UK-Urban Environmental Quality (UK-UEQ) working group is planning to develop guidance for the wind microclimate modelling community to generate wind field outputs suitable for input into dispersion models such as ADMS.

A4.6 Modelling of Non-linear Processes: Complex Chemistry / Radioactivity

The concept of non-linearity applies to a number of aspects of atmospheric dispersion modelling, including chemical and radioactive processes. For certain pollutants, at particular spatial scales, the impact of non-linearity may be neglected, which can simplify, and speed up, dispersion model calculations.

Chemical reactions are non-linear, that is, the products of a chemical reaction depend on the magnitudes of the reactants. Therefore, modelling approaches must allow in some way for the absolute magnitude of concentrations, for example, by modelling a full emissions inventory (for example, for CTMs) or by including estimates of long-range pollutant transport as model input (for example, in local models such as ADMS and AERMOD). Linear approaches, such as using a unit emissions rate combined with an emissions scaling, are inaccurate for pollutants strongly dependent on chemistry, for example, NO_2 at the sub—km scale and $PM_{2.5}$ (particulate matter less than 2.5 micrometres in aerodynamic diameter) at the 10s of km scale. However, modelling full atmospheric chemistry (for example, Master Chemical Mechanism) is computationally intensive and not appropriate for Environment Agency air quality assessments. Other widely used models simplify reaction processes and reaction rates, and consider aggregate (grouped) species which behave in similar ways from a chemistry perspective, for example, volatile organic compounds (VOCs).

Chemical reaction rates commonly depend on meteorological parameters (for example, temperature, solar radiation), so models should use hourly meteorological inputs. However, explicit chemical equations should be modelled at sub-hourly (second) resolution due to the requirement of solving unsteady rate equations.

New fuels and processes may generate pollutants for which chemistry processes are important and complex, for example, generation of toxic nitramines and nitrosamines as a result of CCUS processes using amine solvents.

Radioactive materials decay exponentially, with a decay rate based on the half-life of the isotope. This decay can produce radioactive daughter products which then also undergo their own decay. For many cases, it is the activity generated by the full decay chain which it is important to calculate. Human exposure to this radioactivity needs to be calculated over many pathways, some of which, for example, gamma dose, require details of the whole concentration and/or deposition field even if exposure is only to be calculated at one location. A number of models account for radioactive processes to a greater or lesser extent, including ADMS (Carruthers and others, 1994), AERMOD (Cimorelli and others, 2005), ADMS-STAR (2023) and a number of CTMs.

Deposition processes may also be non-linear (refer to ‘Dry and wet deposition modelling’, section A4.7).

Does the method need more explanation or guidance to ensure it is ‘fit for purpose’?

Dispersion modellers need to be aware of non-linear relationships to avoid the application of ‘linear’ data processes assumptions. Guidance on this in relation to a range of applications would be helpful. For example, differing atmospheric stabilities lead to different dispersion processes and, therefore, resultant pollutant concentrations. As modelled atmospheric stabilities vary hourly, the temporal variation of source emissions leads to a non-linear relationship between pollutant emissions and resultant concentrations, even for those pollutants for which chemical and deposition processes can be neglected. This highlights the importance of including the temporal variation of emissions in modelling studies. Where temporal variations are not known, maximum, rather than average, emissions should be modelled to ensure worse-case concentrations are accounted for.

Source apportionment and emissions scenario modelling methods must consider the non-linear relationship between pollutant emissions and concentrations. For some applications, for example, modelling NO_X and PM at the local scale, near-linearity between emissions and concentrations allows simple modelling of distinct sources, which can be aggregated to predict resultant concentrations. This approach cannot be applied to NO_2 at the local scale and the majority of pollutants at the regional scale due to non-linearities. Different source apportionment methods, specifically ‘potential impacts’, ‘contributions’ and ‘increments’ are the topic of FAIRMODE WG1 on Source Apportionment (Clappier and others, 2022).

Complex chemistry may occur where plumes overlap, for example, at industrial clusters and in urban environments. When modelling these sources, the relative importance of both long-range and local scale pollutant chemical and deposition processes should be considered. Coupled systems may be the most suitable modelling approach where both scales are important (refer to ‘Nested/coupled modelling systems’, section A4.9).

Limitations

As chemical reactions depend on concentration magnitudes, model spatial resolution impacts on chemical process predictions. For example, by virtue of the relatively diffuse representation of 3D emissions in CTMs, peak concentrations are not resolved, for example, near specific industrial sources and at roadside. Consequently, although CTMs model complex chemistry and deposition, short time and spatial scale processes are neglected. The modelling of nitrosamines and nitramines from CCUS is an example where the spatial resolution of the modelled release strongly influences in-plume concentrations due to non-linear chemistry processes.

Possible improvements

As non-linear processes are inherently more complex and computationally intensive to model than linear processes, models make a range of assumptions and simplifications.

Case studies could be developed that demonstrate where non-linear processes are important, and where they are not.

A4.7 Dry and wet deposition modelling

Deposition is the process that removes pollutants from the atmosphere to the surface. While deposition is beneficial in terms of reducing airborne concentrations, it can be detrimental to certain ecosystems if the deposition of a pollutant exceeds the threshold for ecosystem effects (for example, critical loads for nitrogen and acidity; flux-based ozone impact metrics). Accurate prediction of deposition fluxes is, therefore, a critical component of air quality modelling for the purposes of regulation.

Habitat sites of interest include those regulated at EU level (Ramsar, Special Areas of Conservation (SACs) and Special Protection Areas (SPAs)), national level (Sites of Scientific Interest (SSIs) and Sites of Special Scientific Interest (SSSIs)) as well as at local level. Both nutrient nitrogen and acid deposition are important to quantify. Ammonia and NO_X contribute to nutrient nitrogen, while ammonia, NO_X, SO_2, nitric acid (HNO_3), nitrous acid (HONO), and hydrogen chloride (HCl) contribute to acid deposition.

In general, dry deposition processes are assumed to relate linearly to near-ground concentrations. The deposition velocity defines the rate at which the fraction of the near-surface concentration is deposited to the surface. However, for some pollutants such as ammonia, air-surface concentration differences are also important. When stomatal concentrations are higher than those outside the leaf, ammonia can be emitted back into the atmosphere. In addition, a build-up of concentration on outer leaf surfaces can reduce further uptake of a pollutant unless acidic compounds (SO_2, nitric acid, hydrogen chloride) and basic compounds (ammonia) continue to neutralise each other (co-deposition). Compensation points and co-deposition are only considered in few models. It is considered that the wet deposition of SO_2, NO_2 and ammonia is not significant within a short range (AQTAG, 2011).

For dry deposition, in the turbulent region of the atmosphere, gaseous pollutants are primarily deposited as a result of vertical turbulent diffusion. Additionally, very near the ground, gases and small particulates (<100nm) deposit through Brownian diffusion, while larger particulates additionally deposit due to impaction, interception and gravitational settling. Conversely, wet deposition is caused by the washout of pollutants by precipitation and so the wet deposition flux at a particular location is affected by concentration within the whole atmospheric column up to the cloud layer, as well as the precipitation amount.

Deposition modelling is typically not a standalone air quality assessment method. An exception to this is the Concentration Based Estimated Deposition (CBED) model, an inferential modelling system which makes use of an interpolated map of measured concentration in air and precipitation to model the deposition. CBED is run by the UK Centre for Ecology and Hydrology (UKCEH) and is used to assess long-term deposition rates of certain pollutants over the UK at 5km resolution. Deposition processes should be incorporated into any credible, physics-based air quality model.

Local Gaussian models such as ADMS and AERMOD often assume a single dry deposition velocity (per pollutant) over the whole modelling domain, although ADMS also includes an option to account for spatially and/or temporally varying values. Deposition velocities can either be input directly or calculated by the model. In the latter case, ADMS and AERMOD both calculate the deposition velocity via a set of resistance terms, although their specific formulations for these terms differs. AERMOD is more detailed in its calculation but requires more user inputs as a result, including seasonal and land use categories and various pollutant-specific parameters, although defaults are available for common pollutants, and published values also exist (Wesely and others, 2002). Particle size distribution information is also typically required by both models for particulate deposition. In terms of the depletion of airborne concentrations due to dry deposition, ADMS and AERMOD both calculate a depletion factor that increases downwind, while ADMS also includes a normalised adjustment to the vertical concentration profile. Wet deposition calculations are typically based on a prescribed or calculated washout coefficient, a precipitation rate and the column-integrated concentration. The lack of information about the exact location and composition of clouds necessitates a bulk approach.

Over regional scales, deposition is particularly important for correctly modelling atmospheric ozone. In Eulerian grid models such as Community Modelling Air Quality (CMAQ), dry deposition is included as an additional boundary flux condition in the vertical diffusion term of the tracer continuity equation. This acts as a direct sink (or in some cases source) to the concentrations in the lowest layer of the model, and dynamically feeds up to affect concentrations at higher levels. Bi-directional surface fluxes, which can be important for pollutants such as ammonia, as previously mentioned, can be represented through compensation-point models. However, more often the deposition flux is calculated as the product of the spatially varying deposition velocity and atmospheric concentration at the lower boundary. Similar to the local Gaussian models, the deposition velocity is calculated from a network of resistance terms in series and in parallel that depend on surface/vegetation characteristics and aerodynamic surface layer properties. Aerosol deposition additionally accounts for gravitational deposition via the calculation of a settling velocity. Wet deposition due to the removal of gases and aerosols by precipitation is also considered in models like CMAQ via coupling with the cloud module. In-cloud scavenging is modelled using information about the location of resolved clouds and the precipitation rate in sub-grid (convective) clouds. The interception of gases and aerosols by falling precipitation is also considered for convective clouds. However, occult deposition (in cloud or fog) is not considered in the majority of atmospheric models.

Does the method need more explanation or guidance to ensure it is 'fit for purpose'?

The user documentation for most air quality models includes the additional steps and input data requirements when modelling dry/wet deposition.

Current online guidance does not include quantified deposition velocities. Modellers use values from AQTAG06 (2011), which is no longer officially available online.

Limitations

It is difficult to measure dry deposition, so modelling approaches need to be scientifically based and fully verified to ensure accuracy. Model parameterisations of dry deposition processes are based on a small set of deposition measurements and differ greatly between models, highlighting the associated uncertainty. High resolution models (ideally 1km or better) are required to capture orographic enhancements in wet deposition.

Possible improvements

Cumulative assessment should be performed for many studies; the APAS under development by JNCC is intended to facilitate this approach.

Deposition estimates across a wider range of scales could again be achieved via the coupling of regional (for example, Eulerian grid) models to local (for example, Gaussian plume) models.

A4.8 Complex terrain wind field modelling

The term ‘complex terrain’ refers to hilly and mountainous areas, as well as areas with spatially or temporally varying land cover (for example, trees, crops). Wind and turbulence fields in hilly areas are strongly influenced by changes in terrain elevation, while in coastal areas they are influenced by the differing heat fluxes over land compared to the sea. Urban wind field modelling is **not** discussed here.

Wind field modelling is not a standalone air quality assessment method. However, flow and turbulence fields drive pollutant dispersion processes and consequently, meteorological data are required as input to air dispersion models. Where pollutant emissions occur in areas of complex terrain or coastal regions, it is important that dispersion models allow for the spatial and temporal influence the land/coast has on the wind field. In such cases, output from a meteorological model can be used as input to the dispersion model. However, simple approaches, such as the use of meteorological data from a single location, are justified in certain situations, for example:

- where the meteorological data accounts for complex terrain effects
- where the meteorological data accounts for coastal effects
- areas of homogeneous terrain

Meteorological models may be standalone, or they may be integrated within a dispersion model. Wind fields are usually modelled in 3D, at differing spatial resolutions. The horizontal spatial resolution of the meteorological model should be coarser or the same as the spatial scale of the corresponding dispersion model. Table A4.2 summarises the spatial resolution of some commonly used meteorological models. Dispersion models are likely to perform better if the temporal resolution of the meteorological model is the same as the dispersion models (usually hourly). The majority of larger scale meteorological models assimilate measurement data to improve accuracy and generate data that can be used by more than one dispersion model.

Table A4.2: Example meteorological models for complex terrain and coastal modelling

Spatial scale	Grid resolution	Example models
Regional (mesoscale) – global scale NWP	1km or greater	WRF (NCAR Laboratory: Mesoscale and Microscale Meteorology, 2023), Unified Model (Walters and others, 2019)
Mid-range scale	100m – 10s of km	CALMET (Scire and others, 2000), GRAMM (Almbauer and others, 2000)
Fine scale	10s of m – few km	FLOWSTAR (Carruthers and others, 1988)

Meso- and global-scale meteorological models are commonly referred to as numerical weather prediction (NWP) models. The influence of NWP data sets on dispersion modelling is the topic of an ongoing project funded by the Atmospheric Dispersion Modelling Liaison Committee (ADMLC). The study focuses on the impact of applying different grid resolutions of NWP meteorological data in atmospheric dispersion modelling.

Lagrangian Gaussian puff, Lagrangian particle and Eulerian grid models all use 3D spatially and temporally varying meteorological inputs. Gaussian plume models commonly use homogeneous meteorological data as input, but have integrated, parameterised meteorological model features, specifically:

- ADMS and AERMOD derive parameterised 2D boundary layer profiles from input measured or modelled meteorological data
- ADMS incorporates the FLOWSTAR wind flow and turbulence model
- CALPUFF (Scire and others, 1990) includes the CALMET complex terrain module
- GRAL (Oettl, 2016) includes links to the GRAMM wind field mesoscale model

Gaussian models can link to spatially varying meteorological fields within coupled modelling systems.

The ADMLC project ‘Review of atmospheric dispersion in complex terrain’ (Hill and others, 2005) discusses complex terrain modules within ADMS, AERMOD, CALMET and other modelling approaches, including CFD. The report includes an inter-comparison of ADMS and AERMOD in simple terrain, moderate terrain, complex terrain at inland and coastal sites. The effects on model results of changing grid resolution and domain size are also discussed.

Does the method need more explanation or guidance to ensure it is 'fit for purpose'?

There is limited guidance in relation to modelling complex terrain and coastal effects, particularly the latter. Current Environment Agency online guidance encourages modellers to justify their inclusion of terrain effects (Environment Agency, 2023c). In its intensive farm modelling guidance documents, Natural Resources Wales states “the effects of terrain should be considered in accordance with the current recommendation of the dispersion modelling software developer” (Natural Resources Wales, 2019) and the Northern Ireland Environment Agency states that modellers are required to “provide justification for the inclusion or not of terrain treatment and report the source, format and processing of digital terrain data in the model” (Northern Ireland Environment Agency, 2017).

Dispersion modellers should justify their selection of meteorological data inputs and should perform sensitivity testing in relation to the impact of accounting for complex terrain/ coastal effects in the model.

The dispersion model user community would benefit from some guidance in relation to:

- when complex terrain needs to be considered
- how to account for complex terrain in cases where it should be considered
- how to select the best meteorological data location for driving a dispersion model, taking into account whether or not complex terrain/coastal effects are being modelled

The ongoing ADMLC project addresses issues relating to:

a) reliability of NWP data
b) differences in dispersion model outcomes relating to numerical weather prediction (NWP) grid resolution
c) the possibility of double-counting the impact of terrain when modelling using ADMS, including complex terrain effects from FLOWSTAR, driven by NWP data

Limitations

It is unnecessary to model the effects of complex terrain or coastal boundary layers if the model or measurement meteorological data already takes these features into account, and the dispersion model is able to use this information.

Possible improvements

There are published example case study evaluations in the literature, but the outcomes of these could be made more accessible to the user community.

A4.9 Nested/coupled modelling systems

Individual air quality models are only applicable across a limited range of scales. For example, regional Eulerian (grid) CTMs use gridded emissions and are, therefore, unable to resolve the high concentration gradients associated with urban road traffic emissions. Their chemical reaction schemes consider processes that are relevant over long spatial and temporal scales such as secondary aerosol generation, and their use of spatially varying meteorology helps long-range transport predictions. Local Gaussian plume models are typically used for domains between 1 and 50km in size and assume spatially homogeneous meteorology throughout the domain. However, they are able to model dispersion from individual sources explicitly and often include simplified chemistry schemes that only consider fast reactions important on local scales (such as those between NOx, ozone and VOCs), ignoring those that occur on longer time scales. CFD models are able to model plume interactions with individual obstacles such as a block of buildings but their computational expense precludes domains larger than around 1km.

Nested/coupled systems aim to ‘bridge the gap’ between these applicable ranges of scales, therefore harbouring the advantages that modelling at each scale range provides. Examples of when a coupled approach may be required include:

- future scenario modelling: Local models often use measured background concentrations to account for long-range transport into the modelling domain, but these data are not available for future simulations
- source apportionment studies: It may be important to quantify the contribution from various emission sectors, from both long-range transport and local sources, during a particular air quality episode
- spatially varying meteorology: If explicit source modelling is required over a very large urban agglomeration, for example, the assumption of spatially homogeneous meteorology may be stretched

Nested modelling typically refers to the method of using the same regional (grid) model at multiple scales. Increasingly smaller and finer-resolution sub-domains are used to focus in on a particular region of interest, with each sub-domain driven by its parent domain (one-way nesting), with feedback from the smaller to the larger sub-domains also sometimes used (two-way nesting). This method avoids the computational expense of using a fine resolution grid over the entire modelling domain. However, the ratio of grid cell sizes from one domain to the next is typically limited to around 5 to avoid numerical instabilities and so the overall computational expense of nesting from, say, continental to city scale is still large. The so-called ‘spin-up’ time required by these models also increases the computational cost. The use of one model at all scales does, however, ensure consistency. Due to the limitations of the parameterisations used in these gridded models, the upper limit on the attainable grid resolution is in the order of 1km. Therefore, they are still unable to model individual sources explicitly and so cannot be used for roadside concentration predictions, for example. Some examples of modelling systems using nesting across multiple scales include GEM-MACH (Russell and others, 2019), CHIMERE (Siour and others, 2013) and WRF-CMAQ (Chatani and others, 2011).

Coupled air quality systems are typically ‘offline’ systems that use regional-scale meteorological/chemical-transport model inputs/outputs to drive a completely separate smaller-scale model, such as a CFD or Gaussian plume model, within a sub region of the regional model domain.

Due to their computational expense, regional-to-CFD coupled systems are typically only used for very small modelling domains (the CFD domain is often fully contained within one regional model grid cell) and very short modelling periods (typically no longer than one day). The generation of turbulence at the CFD model inlet from the largely laminar incoming regional model flow is also a challenge. These coupled systems are useful for modelling short-term dispersion from one or a small number of sources within a small urban neighbourhood, for example, in an emergency release situation. The CFD models often consider the dispersion of passive tracers only, although there are some examples of rapid chemical reactions being included. Some examples of regional-to-CFD coupled modelling systems include the Integrated Urban Air Quality Modelling System WRF-CMAQ-CFD (Kwak and others, 2015), WRF-OpenFOAM CFD (Zheng and others, 2015) and WRF-LES (Liu and others, 2012).

Coupled systems that use regional gridded models to drive parameterised local (for example, Gaussian plume) models are becoming increasingly common due to their comparatively low computational cost. However, these systems come with their own set of challenges, including the risk of double counting local emissions that are also included in the regional model gridded emissions. This becomes more of an issue as the regional model grid resolution increases. Implementations to avoid double counting include configuring the local model with grid emissions, then deducting resultant grid concentrations from the regional model output to remove short-term local dispersion effects prior to adding in the explicit source contribution (Hood and others, 2018). Other implementation includes using source apportionment in the regional model to separate emissions from within the local modelling domain (Pepe and others, 2016) and extracting concentrations from the regional model that are upwind of the local modelling region as a substitute for rural background concentrations (Kukkonen and others, 2016). Another challenge in coupling regional to local parameterised models is in linking their different sets of chemical reactions. This typically requires a predetermined mapping from the more complex species and reactions used at the regional scale to the simpler ones used at the local scale. Examples of regional-to-parameterised-local coupled systems include the Street-in-Grid model (Lugon and others, 2020), CALIOPE-Urban (Benavides and others, 2019) and ADMS-Urban RML (Hood and others, 2018).

Other types of coupled modelling systems include the nesting of a street canyon model (for example, the Operational Street Pollution Model, (OSPM)) inside a Gaussian model, the driving of local Gaussian models using flow-field output from CFD simulations, and the use of fluctuations parameterisations to predict sub-hourly concentrations within an hourly-average concentration model such as in ADMS. The latter is an example of a temporally coupled system.

Does the method need more explanation or guidance to ensure it is 'fit for purpose'?

The development of coupled systems linking regional to local scale models is a rapidly developing field, and work is still needed to harmonise these developments into clearer guidance. The operation of these coupled systems often requires collaboration between different working groups with specific knowledge of running one ‘part’ of the coupled system, for example, the regional model and the local Gaussian plume model.

Limitations

Nested/coupled modelling systems often require significant computational and time resources to set up, run and interpret the model results. Issues such as the double counting of emissions and linking different chemistry schemes present ongoing challenges in this field, although significant progress has been made in recent years.

Possible improvements

Parameterised local models are often configured to couple with just one or a small number of regional models due to the lack of generality in the inputs/outputs of different regional models. More work could be done to increase the number of compatible regional models, thereby improving the generality of the coupled system.

A4.10 Ensemble modelling

Ensemble modelling involves deriving an ‘ensemble mean’ model result from a range of model outcomes. Methods include the use of multiple different models representing a particular domain, or the same model, representing a particular domain in different ways, for example, minimum and maximum emissions, differing meteorology.

Ensemble modelling approaches provide a modelled concentration and an associated inter-model variability range. Differing metrics can be used to calculate both the concentration and the variability range. Increasing the number of models included within an ensemble improves the reliability of the ensemble model prediction, if all models have similar model performance (for example, with regard to comparisons against measurements). However, ensemble modelling requires additional resources compared to running a single model. The variability range does not necessarily correspond to uncertainty because all models in the ensemble may be using similar inputs.

The Copernicus Atmosphere Monitoring Service (CAMS) (Casciaro and others, 2022) regional air quality forecast is generated using an ensemble modelling approach. Air quality forecasts are generated by 9 European institutions using a range of regional CTM applications. The published forecast at any location is equal to the median concentration over all 9 predictions. A median ensemble model outcome was also calculated from 4 national air quality models as part of Defra’s 2021 Model Intercomparison Exercise (MIE) (Carruthers and others, 2022).

At a smaller scale, simple approaches to ensemble modelling include running both ADMS and AERMOD for a particular site and taking the average or maximum concentrations over both models to represent the model outcome. In this case, the uncertainty associated with the ensemble model outcome is relatively large due to only 2 models being included in the ensemble. Using multiple years of meteorology as input to an air dispersion model as part of an environmental permitting study (Environment Agency, 2023c) is another example of ensemble modelling. ADMS has an option to take an ensemble modelling approach when using meteorological data binned into sectors: when input sectors are greater than 15°, the model executes 5 model runs for each hour, corresponding to the range of wind directions within the sector, and derives a mean concentration.

NWP weather forecasting models often use ensemble approaches by modelling a range of initial conditions; the likelihood (probability) of certain events is derived from the outcomes of the different modelled scenarios.

Does the method need more explanation or guidance to ensure it is 'fit for purpose'?

In terms of local modelling, some ensemble modelling approaches are well established (for example, modelling multiple years of meteorological data), although they are not referred to as such.

Model users are encouraged to undertake sensitivity testing, for example, running models with different inputs (for example, meteorological parameters), or using differing model features (for example, with and without modelling complex terrain). These sensitivity tests are a precursor to ensemble modelling. It may be that, where there is justification for using more than one model input, an ensemble model result should be generated. Guidance could be developed to help model users decide when this approach is justified, acknowledging that additional resources would be required.

Limitations

An ensemble model result will only be more accurate than a single model result if the model inputs used to generate the component results have comparable accuracy. As an example, for the Defra 2021 MIE, one of the component models was excluded from the ensemble calculations at roadside sites because its output resolution was 1km rather than roadside.

An ensemble model result may not be more accurate than a single model result because the accuracy of the result is dependent on the accuracy of the component parts.

Possible improvements

Deriving ensemble model outcomes from different models requires data post-processing. As part of Defra 2021 MIE, the Model Evaluation Toolkit (Stidworthy and others, 2013) was developed to calculate an ensemble result for comparison with measured concentrations. Similar tools could be developed to calculate ensemble results, for example within open air (Carslaw and Ropkins, 2012).

Currently, for the majority of models, setting up and calculating ensemble outcomes from the same model requires data post-processing. Models could be developed to calculate ensemble solutions and associated uncertainty ranges automatically. This would reduce the overhead associated with ensemble modelling in terms of person-hours, although computational resource overheads would remain.

A4.11 Passive samplers

When a passive sampler is introduced into the atmosphere, it samples by molecular diffusion of a gaseous analyte onto an adsorbent medium. The concentration of the adsorbed gaseous analyte is then determined by laboratory analysis, either by chemical analysis (inorganic species, which react with the sorbent) or thermal desorption techniques (VOCs, which adsorb onto the medium). Passive samplers are simple to use, cheap, commercially available and are not dependent on a source of electricity.

Passive sampling can be used to cover a wide range of pollutants, including NO_2, ammonia, VOCs, ozone and SO_2, and environments, including external, internal and personal exposure. Passive samplers are available in 3 different main shapes (Figure A4.1): axial tubes (left), which are deployed vertically and are the most commonly used across the UK, badges (centre) which are worn on the body for personal exposure monitoring, and radial (right), which are deployed either horizontally or vertically.

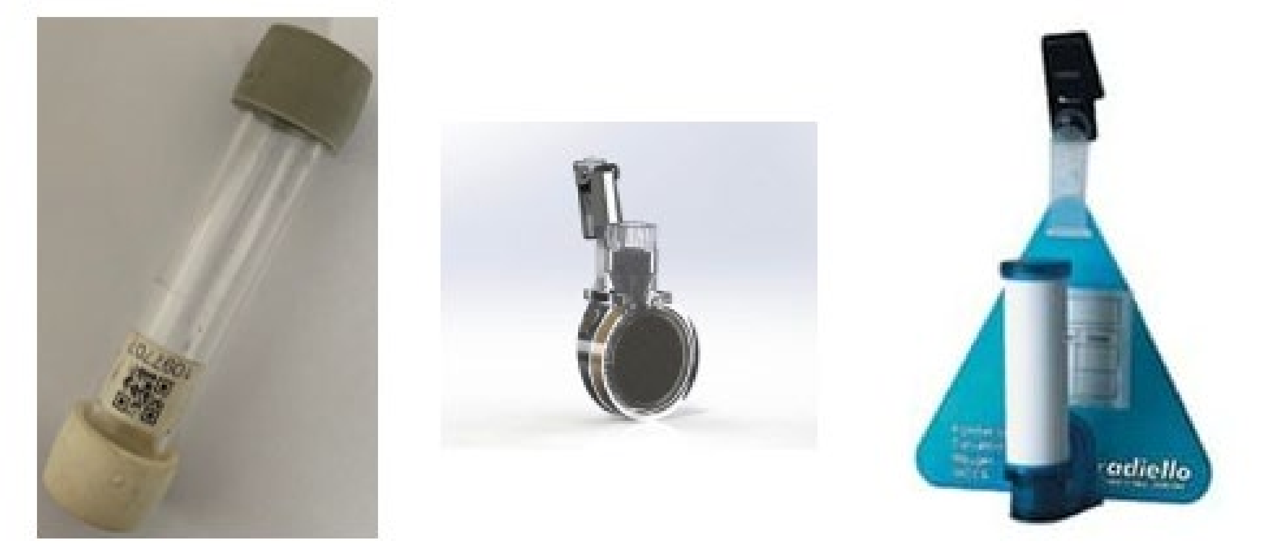


Figure A4.1: Example passive Ssmpling devices: axial tubes (Gradko International), badges (CDL Tecora, 2023) and radial samplers (Radiello, 2023)

Radial passive sampling devices tend to have higher sampling rates owing to a greater surface area of the exposed adsorbent medium, and, therefore, are typically favoured for shorter monitoring periods (~14 days), compared to the axial samplers which are typically used for between 4 and 5 weeks (NO_2) or 4 weeks, in the case of ammonia.

Does the method need more explanation or guidance to ensure it is 'fit for purpose'?

Passive samplers are simple to use and, therefore, require minimal operator training, and the analysis of the adsorbent medium can be carried out by qualified technicians in accredited laboratories. However, it is important that the correct tube type (for example, axial or radial) is selected, as this will affect the sampling duration and the limit of detection or quantification.

There are also European Committee for Standardisation (CEN) standard methods for passive sampling of NO_2 (EN 16339), ammonia (EN 17346) and benzene (EN 14662), which need to be followed for reporting indicative measurements of these pollutants.

A number of manufacturers of passive samplers, for example, Gradko International (2023), provide online technical resources, including datasheets, sampling instructions and frequently asked questions, while Defra and the devolved administrations have published practical guidance online to harmonise the approach to monitoring NO_2 using passive sampling methods (Targa and others, 2008).

Limitations

By their very nature, passive samplers are unable to measure aerosols or particulates, owing to variations in the diffusion processes between gases and particles. Furthermore, as the measured value represents an average time-weighted concentration across the whole monitoring period, the utility of passive samplers is necessarily reduced for assessments of compliance where the relevant objective time period is less than the monitoring period, or for detecting peaks in concentrations arising from industrial locations or point sources where greater temporal resolution is required.

Measurements using passive samplers are subject to a number of different biases (for example, temperature, wind speed, humidity), each of which act independently of one another, and which lead to over- or underestimations in measured concentrations (Heal and others, 2018). Typically, for NO_2 passive samplers, biases arising from exposure are positive and lead to overreads, while biases arising from laboratory analyses are negative and lead to underreads, although laboratory biases have been found to be distributed more uniformly than exposure biases. The overall bias is the sum of each positive and negative bias, and it is often difficult to disaggregate the contribution of each source of bias. One important bias relates to diffusive sampling rate, which is subject to the influence of wind speed, temperature and humidity. Passive samplers have a diffusive sampling rate which is predominantly fixed based on the design of the sampler (Zefon, 2021). If the diffusive sampling rate is too low, there will be insufficient adsorption onto the medium; conversely, where the uptake rate is too fast, the medium can become oversaturated.

Additionally, for monitoring VOCs, sorbent selection is important; if the sorbent is too strong, the pollutant becomes too strongly bound to be released by thermal desorption, while if the sorbent is too weak, the pollutant may not be captured effectively.

Possible improvements

Owing to the effect of wind speed on measured concentrations using passive samplers, manufacturers are currently improving their design to minimise the associated bias. One such improvement involves using 'filters' at the end of the exposed end of the tube to minimise turbulence around the entrance (Martin and others, 2014).

For measurements of ammonia, studies have demonstrated that manufacturer-derived diffusive sampling rates result in high uncertainty in measured concentrations, particularly for higher concentrations (Martin and others, 2019).

Uncertainty

Currently, conventional diffusion tubes for NO_2 only meet the EU Directive uncertainty requirements for 'Indicative measurements' (±25% of a standard reference method). Results have demonstrated that the addition of the filter enables the tubes to meet requirements for 'Fixed measurements' (±15% of a standard reference method) (Butterfield and others, 2021). Mean concentrations derived from triplicate tubes using the filters also demonstrated better precision than conventional triplicate tubes without filters.

A study in 2019 validated the performance of 5 commonly used diffusive samplers for measuring concentrations of ammonia using a controlled atmosphere test facility (Martin and others, 2019). Measured concentrations were used to derive a diffusive sampling rate, which was then compared to the rate used by each sampler manufacturer. The results demonstrated considerable variation in the reported concentrations across each sampler type. However, the recalculation of diffusive sampling rates then enabled improved predictions of concentrations in field comparison results. Subsequently, some manufacturers of passive ammonia samplers have revised their diffusive sampling rates.

A4.12 Low-cost sensors (LCS)

LCS are monitoring devices that measure concentrations of pollutants in the atmosphere in real-time, but that are available at much lower purchase cost, are typically more portable, have potentially better time resolution ability (Frederickson and others, 2022; Candice Lung and others, 2018), and are generally easier to operate than reference equivalent monitors.

In recent years, the sensor industry has undergone rapid development, and, therefore, there is a wealth of commercially available sensor products produced by a variety of manufacturers. Correspondingly, there has been an exponential increase in the number of studies using LCS, as demonstrated in Figure A4.2 by the volume of published literature referencing 'LCS' and 'air quality' on PubMed (National Library of Medicine, 2023).

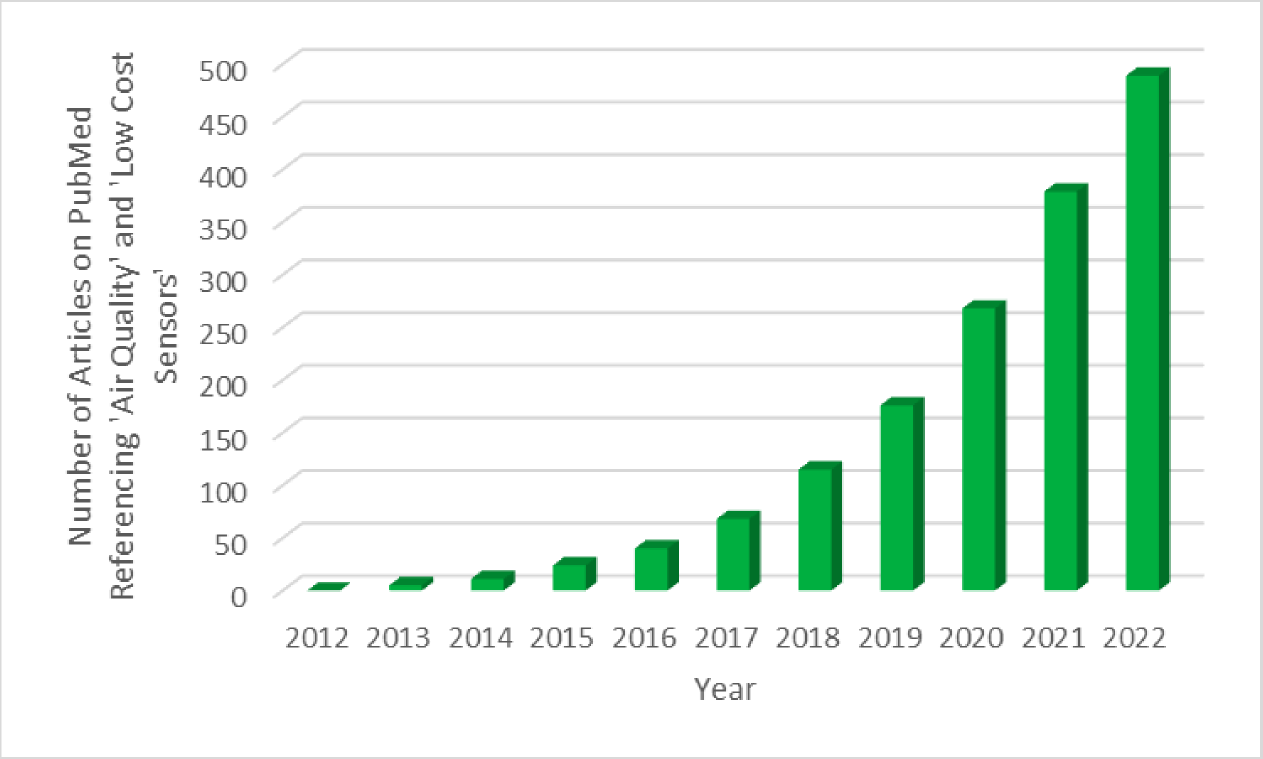


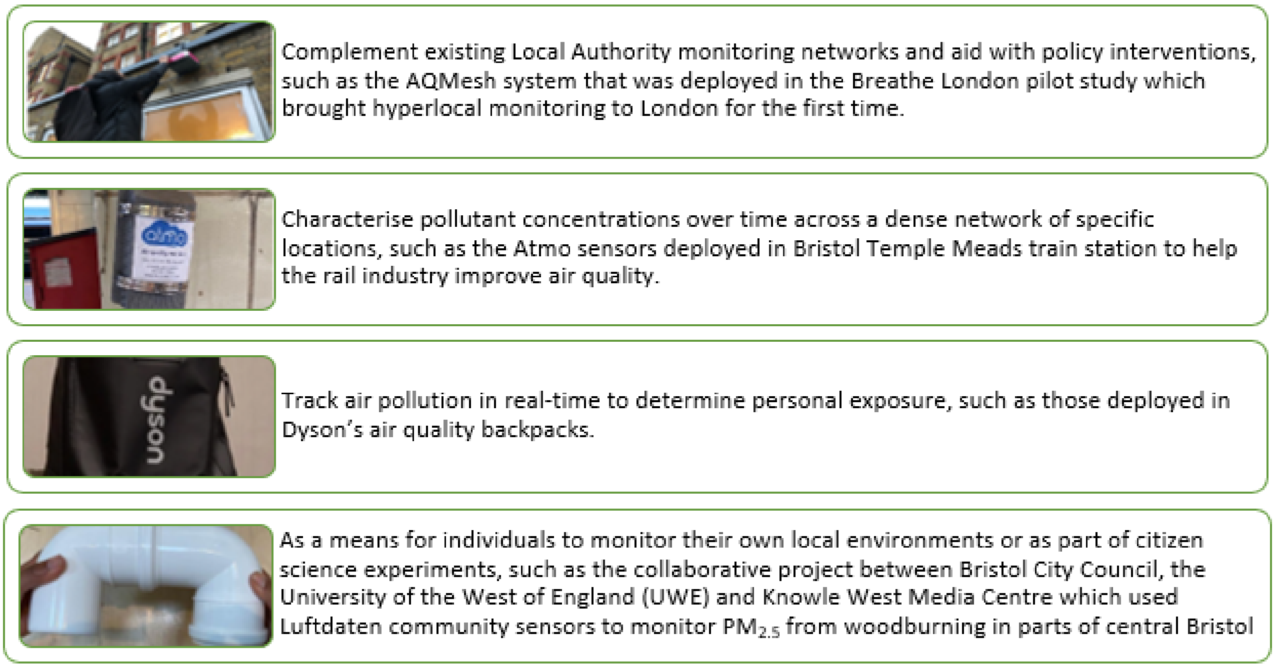
Figure A4.2: Number of Articles on PubMed Referencing ‘air quality’ and ‘low-cost sensors’ between 2012 and 2022 (National Library of Medicine, 2023).

LCS typically comprise several different sensor types depending on the pollutant(s) of interest:

- Particulate matter is often measured using optical counters comprising a laser beam and photodiode. As particles move through the beam, the light is scattered and detected on the photodiode, which is converted into an electrical current. Particle size is then determined based on the magnitude of the voltage pulse using a calibration curve. These types of systems use an assumed particle distribution to convert $PM_{2.5}$ data to PM_{10} (particles less than 10 micrometres in aerodynamic diameter), and, as a result, optical sensors are more accurate when composition is known, since the instrument response function is less ambiguous.
- Carbon monoxide (CO), NO_2, NOx, nitric oxide (NO), SO_2, ammonia and ozone are often measured using electrochemical sensors, which consist of electrodes and an ion conductor or electrolyte reservoir. When the gas of interest interacts with the electrodes, redox reactions occur which generate electrical signals proportional to the concentration of the gas.
- VOCs are measured using either electrochemical sensors, metal oxide (such as tin dioxide) semiconductors, flame ionisation detectors, or mini gas chromatography machines. Using metal oxide semiconductors, changes in measured currents are recorded when the metal oxide layer is heated and exposed to VOCs.
- Carbon dioxide and CO are measured using non-dispersive IR cells, which determine concentrations based on the absorption of certain wavelengths of light.

The potential of LCS is exciting to many sectors in the air quality industry since they can be deployed in vast numbers, thereby offering greater insight into sources and patterns of air pollution. They also provide increasing opportunities for air quality monitoring to a greater proportion of the population, potentially reducing social disparities. The sensors do not, however, evidence equivalence with reference monitors. Therefore, there is doubt among the air quality community as to their widespread use, with respect to accuracy, reproducibility and comparability, particularly with regard to regulatory roles and compliance and the potential for resulting prosecutorial action. Measurements using LCS are often subject to drift and cross-interference with pollutants that are present simultaneously and which may vary with time. Notwithstanding the above, in some instances, where it is more important to understand the cause/solution of air pollution (such as identifying hot spots, raising public awareness and complementing existing monitoring programmes) rather than determine the absolute concentration of a substance, the ability to operate a dense network with high time-resolution is invaluable. However, there is still a requirement to ensure that variability between sites and throughout time is minimal.

Owing to their advantages over other monitor types, LCS have been used for a number of studies, including, but not limited to, those set out in Figure A4.3.



Complement existing Local Authority monitoring networks and aid with policy interventions, such as the AQMesh system that was deployed in the Breathe London pilot study which brought hyperlocal monitoring to London for the first time.

Characterise pollutant concentrations over time across a dense network of specific locations, such as the Atmo sensors deployed in Bristol Temple Meads train station to help the rail industry improve air quality.

Track air pollution in real-time to determine personal exposure, such as those deployed in Dyson's air quality backpacks.

As a means for individuals to monitor their own local environments or as part of citizen science experiments, such as the collaborative project between Bristol City Council, the University of the West of England (UWE) and Knowle West Media Centre which used Luftdaten community sensors to monitor $PM_{2.5}$ from woodburning in parts of central Bristol

Figure A4.3: Applications using low-cost sensors (Frazer-Nash Consultancy, 2021; Dyson, 2022; The Newsroom, 2021), Photo credit AQ Mesh: Nick Martin

Does the method need more explanation or guidance to ensure it is 'fit for purpose'?

Results from LCS need to be treated with care and understood in context. To manage the inherent uncertainties associated with LCS, suitable guidance can help the public and researchers to critically evaluate sensor performance and guide the decision-making process on the most appropriate and robust uses of any subsequent data.

Defra's Air Quality Expert Group (AQEG) has provided advice on LCS (Defra, 2018), further signposting the US EPA's 'Air Sensor Guidebook', which aims to help those interested to collect and analyse sensor data correctly (United States Environmental Protection Agency, 2022). The US EPA updated the guidebook in 2022 to reflect new information, included sensor performance guidance, determining the purpose for monitoring and how to coordinate a monitoring study (Clements and others, 2022). Similarly, the European Committee for Standardisation (CEN) has published a technical specification (CEN/TS 17660-1:2021), which specifies the general principles for the classification of LCS for monitoring gaseous compounds (European Committee for Standardisation (CEN), 2021a). Currently, Defra and the British Standards Institute are in the process of developing a publicly available specification for low-cost sensors, which will seek to give advice about how to use LCS in certain situations.

Further guidance and understanding are also needed to reinforce the importance of standardisation against reference monitors. While co-location studies are a valuable asset, such standardisations may only be valid for a unique set of circumstances, therefore, it is critical that any evaluation process considers the suitability of the test environment. For example, European monitors standardised in Mediterranean climates may not be suitable for monitoring programmes in the UK due to different humidity profiles. Of relevance is the deployment of 'Air Quality Sensor Farms' (Urban Flows Observatory, 2020) to compare the performance of multiple different sensor types, between both different sensor manufacturers and with a reference sensor. The sensor farms are exposed for prolonged periods of time to experience a range of climatic conditions and corresponding range in pollutant concentrations.

Additionally, given the extensive range of LCS products available, performance criteria for networks need to be better defined to allow multiple equipment types to be used and ensure that measurements are comparable across different sensor types and brands.

Additional guidance is also available within FAIRMODE cross-cutting Task 6 (European Commission, 2021a), which focuses on:

- exchanging concepts and best practices about the integration of sensor network data in air quality mapping methods
- exploring how air quality modelling can contribute to the exploitation and validation of air quality sensor network

Studies have commented that the use of global performance metrics, including root mean square error (RMSE), can obscure the nature of uncertainty associated with LCS and subsequently the effect of the uncertainty on any monitoring campaign (Diez and others, 2022). This is because global performance metrics represent an 'average' over the entire data set, rather than focusing on measurement errors across the entire concentration range. Ultimately, the use of global metrics to describe uncertainty mask errors and features (such as step changes or non-linearities), often leading to the selection of devices that are not fit for the purpose of the monitoring campaign.

Limitations

A review conducted by the World Meteorological Organisation (Castell and others, 2020) into the performance of LCS identified several common issues, including:

- drifts in baseline measurements
- high sensitivity to changes in atmospheric humidity and temperature
- production of false signals if other air pollutants are present in high concentrations
- cross-interference from other pollutants, including ozone and water

CEN/TC 264 Working Group 42: Part 2 (European Committee for Standardisation (CEN), 2021b) has documented that the standardisation of particulate matter (PM) sensors is difficult, noting that reference equivalent measurements depend on the location and type of monitor (gravimetric and automated methods such as tapered element oscillating microbalance (TEOM) instruments). Particle size is calculated based on calibration curves which assume a certain particle distribution, and, therefore, can differ across locations and sources; for example, some sensors are better at measuring course particulate matter fractions, such as those that derive from cement factories.

While the purchase prices of LCS are typically low, this is not usually accompanied by any access to the data; subscription costs can, therefore, result in additional charges, particularly where there are many nodes in a network.

Possible improvements

Technical specifications are often developed through discussion (for instance, identifying what tests are needed and associated costs), rather than directly through assessment. The balance between the cost and type of testing is important, however specifications based on field measurements are invaluable. The Strategic Priorities Fund Clean Air Quantification of Utility of Atmospheric Network Technologies (QUANT) project aims to quantify sensor accuracy and inform sensor calibration methods (UK Research and Innovation, 2022). The project will enable the delivery of a real-world open and traceable assessment of commercial LCS which will serve to improve measurements using LCS.

The C40 cities, who are a global network of mayors taking action against climate change, have prepared a report highlighting 11 cities that have deployed LCS to monitor air quality. As part of the report, there are a number of recommendations for sensor technology based on challenges recorded by the 11 cities taking part (C40 Cities, 2022). The recommendations included:

- clear protocols for co-location and frequency of calibration
- recent and reliable data on sensor accuracy under local conditions
- solutions to energy supply disruptions and city-specific conditions

- estimating the useful lifetime of sensors
- robust and responsive customer support
- offer training to increase local staff capacity
- anticipate and reduce e-waste from sensors
- support with project-level budgeting
- guidance on data sharing and data management platforms

The literature also presents a variety of approaches for improving the accuracy of unprocessed sensor data, including calibrations using co-locations with reference instruments, in-field calibrations, and machine learning (ML) techniques (Peters and others, 2021).

In order for data from LCS to reliably complement existing networks for compliance purposes, the uncertainty surrounding measurements must be reduced and mirror the uncertainty range associated with reference (15%) and indicative (25%) monitors.

Uncertainty

The sources and nature of all the errors are unknown or difficult to quantify across all possible end-use applications, meaning estimates of measurement uncertainty associated with LCS as a whole are difficult (Diez and others, 2022). Ultimately, performance criteria are specific to the technology type, vintage, manufacturer, and environment type, and, therefore, caution should be exercised with extrapolating uncertainty values across to other sensor types and environments.

Numerous studies have, however, attempted to document the uncertainty associated with LCS (Peters and others, 2021; Giordano and others, 2021). One such study (Peters and others, 2021) evaluated the uncertainty associated with the 100 NO_2 electrochemical sensors deployed as part of the Breathe London project using co-location measurements with reference sensors, and derived a root mean square error (RMSE) of 35%. The study also identified that there were infrequent multi-week periods of poor performance, but that bias associated with the sensors varied seasonally, peaking during the summer months.

A4.13 Reference monitors

Reference monitors, a selection of which are shown in Figure A4.4, are sophisticated air quality monitoring instruments that comply with the minimum performance requirements as set out in the Air Quality Directive (The European Parliament and the Council of the European Union, 2008). The Directive also has minimum data capture thresholds that monitors must meet, which include an allowance for periods of planned maintenance, such as calibrations, audits and servicing. The EU has published a series of standard methods (CEN reference standards) that specify the tests and requirements for analysers to achieve, based on laboratory and field studies. In the UK, the Environment Agency has implemented the MCERTs monitoring certification scheme (Environment Agency, 2023d), which, with the exception of instruments for monitoring particulate matter, is generally aligned with the CEN reference standards.

Where a reference method is provided for a gaseous pollutant, it must comply with the relevant MCERTs performance standard. For automatic PM_{10} devices, the MCERTs performance standard has been tailored to reflect the typical UK PM_{10} composition. Alternative methodologies and techniques can, however, be followed if they can demonstrate ‘equivalence’ with a reference method. For a method to be described as ‘reference equivalent’, the measurement uncertainty must be within 15% (for gaseous analysers) and 25% (for particulate analysers) at the relevant limit value, and it must be able to be shown to meet the data capture requirements (90% for all pollutants, except ozone during winter when the requirement is 75%).

Figure A4.4: Reference monitors: Marylebone roadside site, Bristol St Paul’s urban background site and Bush Estate rural background site (Defra, 2023d).

In alignment with the CEN reference standards (2005) set out in the Air Quality Directive (The European Parliament and the Council of the European Union, 2008), gaseous pollutants in ambient air are drawn in through an inlet and analysed using ultraviolet (UV) absorption (ozone), chemiluminescence (NOx/NHx), UV fluorescence (SO_2) and IR absorption (CO). For particulate matter, the reference method involves a gravimetric technique which is based on manually weighing the sample; this precludes the ability to monitor continuously. The gravimetric technique can also result in underestimations due to evaporation of semi-volatile components, while the condensation and evaporation of water can also affect measurement data (Air Quality Expert Group, 2005). Therefore, measurements of particulate matter favour using reference equivalent methods, including tapered element oscillating microbalance (TEOM) with filter dynamics measurement system (FDMS), beta ray attenuation and optical particle size spectrometry. For ammonia, there is no recognised reference method, therefore, many experts consider the denuder technique to be the most reliable method to measure ambient ammonia concentrations (Martin and others 2019). Monitoring methods and reference standards are also available for a number of pollutants associated with industrial processes, such as:

- heavy metals (analysed using inductively coupled plasma mass spectrometry)
- toxic organic micro-pollutants (TOMPs) (analysed using mass spectrometry and gas chromatography techniques)
- polycyclic aromatic hydrocarbons (analysed using gas chromatography mass spectrometry)
- volatile organic compounds (VOCs) (analysed using gas chromatography)

Measurements are collected by the monitors at regular intervals (for instance, every minute), and can then be processed to give rise to sub-hourly (for example, 15 minutes), hourly and daily averaged concentrations. Data are then uploaded online instantaneously using telemetry. The Air Quality Expert Group (AQEG) has previously recommended that data were collected and stored at higher measurement frequencies (Air Quality Expert Group, 2015).

In order to ensure that the data produced are accurate and reliable, reference monitors undergo a rigorous quality assurance (QA) and quality control (QC) process, involving biannual audits (including intercalibration) and quarterly data ratification, alongside regular maintenance (Defra, 2016).

Does the method need more explanation or guidance to ensure it is 'fit for purpose'?

Regulatory bodies responsible for monitoring compliance have issued documents related to the requirements for reference monitors as well as technical guidance notes, for example:

- Defra’s guide for local authorities for purchasing air quality monitoring equipment (Mooney, 2006)
- The Environment Agency’s guidance on developing monitoring strategies (Environment Agency, 2011)
- Defra’s QA/QC procedures document for air quality monitoring (Defra, 2016)
- Defra’s summary on EU standard methods for monitoring in the UK (Defra, 2023e)
- The regular Automatic Urban and Rural Network (AURN) annual technical reports (Ricardo, 2022)
- The Environment Agency’s guidance on performance standards (Environment Agency, 2023e)

A study of equivalence comparisons for particulate matter demonstrated that the statistics were highly influenced by data recorded at high concentrations, and that the equivalence comparisons are sensitive to particle composition (Allan and others, 2022). As such, the UK embarks on a programme of continued particulate matter equivalence studies to ensure that monitors can still be classed as reference equivalent, and to identify changes in pollutant composition that may require additional guidance to ensure suitable techniques are used.

Limitations

Levels of air quality can vary within a few metres for a multitude of reasons, including localised sources, differences in topology and the built environment, and the presence of microclimates affecting the weather. The sparse distribution (relative to the potential for dense sensor webs) of reference monitors and their non-mobile nature, while suitable for characterising local air quality, introduces the assumption of a homogenous environment to extrapolate concentrations from one location to another, and may potentially prevent the small distinctions (such as those originating from stacks) from being detected.

The size (often bulky), cost (expensive), and power requirements (require continuous power supply to operate) associated with reference standard monitoring equipment can also be prohibitive to their widespread use. In some instances, planning permission is also required to install the monitors, which can restrict placement.

To meet the stringent QA/QC requirements, reference monitors are required to undergo regular audit processes, which can lead to loss of data for a period of time; provisions are made in the EU guidelines for 5% instrument downtime, equivalent to approximately 2.5 weeks. Three main data issues are commonly identified during the annual audit process (Ricardo, 2022): poor performance of some analysers which resulted in a change of manufacturer, degradation of the equipment (such as seals) leading to leaks in the monitors, and aging monitors leading to poor performance.

Possible improvements

A main avenue of improvement relates to the facile integration of reference monitors with other monitoring devices (such as low-cost sensors (LCS)) and with models. While data from reference monitors are continuously made available online, they are averaged over different temporal resolutions to devices such as LCS, which can provide data on a second-by-second basis (see ‘Low-cost sensors’, section A4.12). As such, an important area for improvement is the integration of reference data with other techniques.

Different networks, such as those operating as part of local air quality management (LAQM) regimes, may also use reference methods. However, they do not necessarily follow the Air Quality Directive compliance criteria, particularly with respect to QA/QC requirements. As such, reference methods should be aligned, and differences in procedures highlighted as part of any sharing of data in a single central repository or across different methods.

Reference monitors are also integral to the development of LCS. Field co-locations to develop calibration models for correcting data need to be carried out in representative locations, which can be potentially limited by the geographical spacing of reference monitors across the UK.

A further barrier to monitoring extensively using reference monitors is their cost. ‘Near reference’ monitors have recently, however, been raised as a potential alternative, offering an intermediate solution between high cost/high quality reference monitors and the low-cost sensors that have disputed levels of accuracy (Moroni and others, 2022). Data from near reference monitors have been shown to be of sufficient accuracy (for example, for NO_2, within the uncertainty range of reference (15%) and indicative (25%) monitors) and quality to complement existing networks, but at vastly lower cost.

Uncertainty

To meet the definition of a reference monitor, the expanded measurement uncertainty must not exceed 15% (for gaseous analyser measurements) or 25% for particulate matter instruments. The magnitude of the uncertainty level must, however, be borne in mind when comparing measurements against objectives and limit values. In the case of particulate matter, as the UK strives to meet the new value of 10µg/m^3 as an annual mean, within the reference monitor uncertainty bounds, the true value could be 7.5µg/m^3 to 12.5µg/m^3, which covers the range of concentrations widely seen across the UK. Small changes to concentrations realised through targeted policy action may, therefore, be masked by the uncertainty in the true value, limiting the value of monitoring.

In 2021, only 4 sites that form part of the AURN did not meet the necessary uncertainty requirements (Ealing Horn Lane (PM_{10}), Horley (NO_2), Newcastle Centre (PM_{10}) and Southend-on-Sea (NO_2)) (Ricardo, 2022). The reasons for data loss at the monitoring stations were predominantly due to instrument or air conditioning faults, response instability or problems associated with the replacement of analysers and infrastructure.

A4.14 Urban supersites

Supersites comprise advanced air quality monitoring instruments that are able to measure a range of pollutants and meteorological data. Supersites offer a large range of pollutant measurements in a single location, including nanoparticles, ammonia and volatile organic compounds (VOC), as well as enabling a wide understanding of the sources and processes that lead to poor air quality, such as changes to sources of NO_2 (for example, as a result of moving toward net zero modes of transport), trends in ammonia emissions arising from changes to farming practices and identifying the changes in the emissions of VOC precursors to ozone formation, notably biogenic VOCs, that may increase as a result of the government's latest tree planting strategy (Environment, Food and Rural Affairs Committee, 2022). Supersites also enable online particle composition characterisation, which permits receptor modelling activities for particulate matter apportionment, such as for non-exhaust emissions and woodburning.

Currently, there are static urban supersites located in background locations in 3 main English conurbations: Birmingham, London, and Manchester (see Figure A4.5). The sites were installed between 2018 and 2019 as part of a National Environment Research Council (NERC) funded project. In 2021, 2 mobile supersites, in the form of an electric mobile van (see Figure A4.5) and a container mounted on a trailer, were established. These complement existing mobile facilities used by the University of York, Imperial College London and the UK Centre for Ecology and Hydrology (UKCEH), installed with monitoring equipment similar to those used at static supersites, albeit with marginally different instrument payloads. Defra also has 2 well-established rural supersites (Auchencorth Moss and Chilbolton), commissioned as part of the European Monitoring and Evaluation Programme (EMEP). However, these are focused on regional chemical transport and transformation processes rather than the impacts of local sources of pollution. A roadside supersite is also installed on Marylebone in central London.

Figure A4.5: University of Manchester supersite (University of Manchester: Centre for Atmospheric Science, 2023) and University of Birmingham mobile supersite (Atmospheric Measurement and Observation Facility, 2023).

Measurements from supersites have been linked with satellite observations to assess how well the latter computes ammonia concentrations (Marais and others, 2021). These measurements are also used to calibrate low-cost sensors (such as the Breathe London network), and have been used to test sensors for hazardous chemical releases (such as by the Defence Science and Technology Laboratory (DSTL)). In addition, data from supersites is regularly shared with the Meteorological Office to help with forecast modelling, and as part of Defra’s air pollution forecasting.

Detailed atmospheric composition data from supersites are valuable for quantifying impacts from existing and emerging sources, such as microplastics from tyre wear. Data from supersites have also been used to provide the basis for mapping cooking aerosol across the country or coupled with roadside monitors to calculate non-exhaust emission factors. As the source of the pollutants, for example $PM_{2.5}$, can be resolved, supersites enable policy interventions to be more targeted, and help with minimising inequalities in exposure.

Article 10 of the Draft EU Directive requires the installation of supersites to measure certain species such as ultrafine particles (UFP), ammonia and heavy metals, while the World Health Organization (WHO) has recommended in recent reports that black carbon and UFP should be monitored. Therefore, the EU is currently proposing to include the Aerosols, Clouds and Trace Gases Research Infrastructure (ACTRIS) supersite network into the Air Quality Directive update. In the United States, a $12 million grant is helping to establish the Atmospheric Science and Chemistry Measurement Network (ASCENT), which will be aligned to the ACTRIS protocols, including instrumentation, data quality assurance and data sharing. While the UK no longer forms part of the EU, the UK could also follow these protocols.

Does the method need more explanation or guidance to ensure it is 'fit for purpose'?

Since the supersites consist of a number of complex monitoring techniques, such as aerosol chemical speciation, X-ray fluorescence and scanning mobility particle sizers, they are currently managed by academic researchers. If the Environment Agency were to include urban supersites, additional resource, such as training, guidance or outreach activities may be required to enable the measurements to be processed and analysed (using processes such as Positive Matrix Factorisation (PMF)) and ensure the correct maintenance of the internal equipment. Alternatively, the management could be contracted to universities or research centres familiar with operating supersites.

Limitations

Supersites are highly expensive; the National Environment Research Council (NERC) invested £4.3 million as part of the initial installation stage, followed by an additional £1.3 million to introduce the 2 mobile supersites.

Supersites are also spatially limited since they often have a reasonable footprint and infrastructure and energy requirements. The information collected by a supersite is also constrained to a specific location, and, while the instrumentation associated with the supersite enables a broad range of pollutants to be measured, the measurements only represent that individual location, which may not necessarily reflect where targeted action is required, or where policies need to be reviewed to enhance air quality. For example, most of the static urban supersites are currently installed in background locations, and, therefore, they offer minimal insight into industrial or roadside environments that are associated with higher pollutant concentrations.

Possible improvements

The current urban supersites do not cover a range of different environments as they are all mostly located in urban background locations, apart from during the short-term campaigns using the mobile supersites and the Marylebone Road site. These supersites do not cover the locations where social inequalities may be greatest, and do not all cover where air quality is poorest. Therefore, the network could be expanded to enhance the geographical coverage and offer a broader representation of different environments.

Uncertainty

The supersites are installed with state-of-the-art instrumentation that measure with high time resolution. They undergo periodic calibration to reference standard equivalence and data are ratified to minimise the degree of uncertainty and identify any issues with equipment that may affect outputs. On this basis, measurement data derived from supersites are associated with low levels of uncertainty.

It should, however, be recognised that supersites do not have the same formalised accountability chain as the compliance metrics require. Protocols to ensure standardised calibrations and auditing processes are in varying stages of development within ACTRIS.

A4.15 Mobile air quality monitoring

Mobile methods involve using measurement instruments for short monitoring campaigns in temporary locations, before moving to a different location. The campaigns may be short, and last for hours or days, or may be longer, lasting several months. Monitoring devices have been deployed on unmanned aerial vehicles (UAVs), road vehicles and aircraft. As air quality targets move toward exposure-based approaches, mobile networks may become more relevant.

Mobile monitoring methods have a variety of uses, including to complement existing static networks and fill gaps in understanding, monitor air quality along stretches of roads to manage the impact of road traffic emissions on the surrounding environment (Aeroqual, 2021), and to monitor industrial accidents and natural disasters such as wildfires (Cummings and others, 2021; Nance, 2021). Methods used on UAVs or aircraft can be used to monitor areas with poor accessibility at ground level.

Researchers in Thailand (Duangsuwan and Jamjareekulga, 2020) have developed the ‘drone for real-time air pollution monitoring (Dr-TAPM)’ (see Figure A4.6), which is able to monitor concentrations of a number of pollutants (including ozone, NO_2, PM and SO_2) using ‘off-the-shelf’ sensors and transmit the data in real-time. Researchers in Canada and Nigeria have developed the utility of the drone further, and implemented on-board pollution abatement systems that automatically release scrubbers when the drone detects concentrations of NO_2 above recommended levels (Rohi and others, 2020).

The University of Birmingham, as part of the NERC funded UK Air Quality Supersite Triplets (UK-AQST), manages 2 sustainable mobile supersite platforms (one electric van (see Figure A4.6), one trailer) that augment the static supersite network. When deployed, these are positioned relative to the static supersites at rural and roadside sites and enable researchers to better understand the relationship between traffic and urban emissions, as well as the transmission of pollutants.

Other aerial instruments include the use of balloons (such as ozonesonde measurements) and aircraft (such as those used as part of the Regional Atmospheric Measurement Modelling and Prediction Program in the United States) (see Figure A4.6). Measurements collected from aircraft have previously also been used by the National Aeronautics and Space Administration (NASA) to improve satellite measurements, since the aircraft can fly in ‘spirals’ and measure the vertical distribution of pollutants.

Figure A4.6: Dr-TAPM UAV (Duangsuwan and Jamjareekulga, 2020), University of Birmingham supersite van (Atmospheric Measurement and Observation Facility, 2023), Ozonesonde balloon measurements (National Oceanic and Atmospheric Administration, 2017) and Aircraft (Dickerson, 2015).

Does the method need more explanation or guidance to ensure it is 'fit for purpose'?

Recent technological advances make mobile monitoring a realistic option. However, the air quality equipment used should meet certain standards to ensure it is suitable for the monitoring programme. This particularly applies to the use of UAVs, since they have weight limitations and are often mounted with low-cost sensors, the quality of which may vary from user to user.

The purpose of the mobile monitoring campaign also needs to be well defined. For example, if a robust assessment of the monitoring data is required, calibration and data quality assurance may need to be integrated into the monitoring period to ensure that the returned data is of sufficient quality. However, this may not be the case if the mobile programme is for reconnaissance purposes only.

Limitations

Currently, many mobile units are not equipped with fast ammonia sensors, therefore, they often preclude the ability to measure concentrations. This minimises their use for monitoring associated with emissions from the movement of agricultural waste and fuel (for example, for shipping).

Where measurements from aerial devices have measured a column of air, or through a pathway, they are not analogous with legislative requirements which are based on concentrations at fixed points.

The vehicles for carrying the mobile instruments often have emissions associated with their own operation, notably fuel combustion from aircraft, requiring careful consideration of sensor inlets. Issues with interference from other sources, such as when ships are used as launch platforms, can also occur. Where interference is detected, contaminated data are often removed. UAVs also have limited endurance properties, depending on the power source, although several have explored the possibility of mounting solar cells to resolve issues with power consumption (Rojas and others, 2015).

While UAVs do not have any direct emissions themselves, they can struggle to carry heavy monitoring equipment, and are subject to flight restrictions. Users are also required to apply for an operator ID from the Civil Aviation Authority (Flying drones and model aircraft, 2023), since the weight is likely to exceed 250g. In addition, campaigns using UAVs are limited by environmental conditions, such as high wind speeds when they cannot be operated. Onboarded sensors can suffer from electronic interference (Rohi and others, 2020) and are often developed and calibrated for stable conditions, therefore, they are highly sensitive to changes in the environment.

Since mobile methods are used for short periods of time, they do not provide any information about continuous long-term trends, while the scale of the deployment, and subsequent data coverage, can also be limited by the cost of the observation instruments onboarded onto the vehicle.

Possible improvements

A successful mobile monitoring campaign requires appropriate instrument selection, a well-planned and executed experiment design, a thorough quality assurance plan, and use of appropriate statistical techniques.

Uncertainty

The level of uncertainty of mobile methods is dependent on the type of instrument used. For example, the mobile supersites meet the same data standards as the static supersites, and, therefore, are associated with low uncertainty. Contrastingly, drones used with low-cost sensors may be associated with higher levels of uncertainty, particularly if the sensors have not been calibrated correctly.

A recent study (Whitehill and others, 2020) concluded that characterising instrument performance in the mobile context is challenging, yet necessary, to define quality assurance requirements, albeit it concluded that there was parity in uncertainty between mobile and static co-locations.

A4.16 Ground-based remote sensing measurements

Remote sensing of air pollutant concentrations involves processing infrared (IR) and/or ultraviolet (UV) radiation to detect the presence of specific atmospheric species. Only a subset of pollutants is detectable in the IR range; these include greenhouse gas pollutants. There are 2 main types of ground-based remote sensing:

- **active**, where a source of radiation is emitted and reflected back to a sensor. Path-integrated or range-resolved concentrations can be calculated
- **passive**, where the sun is used as an external source of radiation either in direct solar measurements or through measurements of scattered light. Generally, total atmospheric column concentrations are calculated using an upward pointing optical

spectrometer. Similar to satellite remote sensing, the direct solar methods rely on clear skies

Ground-based remote sensing of Environment Agency regulated sources is commonly used as part of the process for estimating source emissions, for example, from industrial and waste sources. A necessary part of this process is to measure in-plume concentrations; emissions are then estimated, for example, using inverse modelling or tracer gas approaches.

The National Physical Laboratory has used its Differential Absorption Lidar (DIAL) remote sensing equipment for a number of applications. This includes remote measurements into inaccessible, hazardous or elevated areas; wide area surveys of diffuse sources including methane from landfill sites (Innocenti and others, 2017); measurement of total industrial site emissions, including flares (Environment Agency, 2019) and tanks; boundary fence monitoring; identification and quantification of leaks and fugitive emissions; plume tracking and source identification from complex industrial plants; and environmental impact assessments.

The DIAL technique uses a laser source of tuneable wavelength (UV or IR) that is transmitted over the measurement region. A small fraction of this light is scattered back by aerosols and particulates that are present in the atmosphere. This is collected with a telescope and a fast, sensitive detector. The extent of the absorption is known from accurate laboratory data, and this enables the concentration and spatial distribution of the atmospheric pollutants to be determined. DIAL can collect real-time data for gaseous species with characteristic absorptions from the UV through to the mid-IR spectral region, including methane, ethane, ethene, ethyne, general hydrocarbons such as petroleum and diesel vapours, hydrogen chloride, benzene, toluene, SO_2, NO and NO_2.

Differential Optical Absorption Spectroscopy (DOAS) systems can be used in either direct or passive configurations, but typically work with UV/visible light (UV/vis) measurements of scattered sunlight to calculate range-integrated concentration fluxes. Examples of applications of these methods for assessing industrial source emissions include (Johansson and others, 2014) and (Mellqvist and others, 2007). In these examples, DOAS are used alongside Solar Occultation Flux (SOF) systems, which use Fourier transform infrared (FTIR) spectroscopy of direct sunlight. Another example is the MAX-DOAS instrument that performs multi-axis UV/vis measurements of scattered light to assess the spatial distribution of species such as NO_2, O_3, formaldehyde, glyoxal and water vapour (Oxford Instruments, 2023).

Tunable diode laser absorption spectroscopy (TDLAS) is a well-established active open path method that can be used to detect pollutants, including hydrogen sulfide (H_2S), methane, CO, CO_2, ammonia, hydrogen chloride (HCl) and hydrogen fluoride (HF) (Lackner, 2007). Applications include continuous emissions monitoring and process control.

Out of scope for this report is a discussion of the extensive use of remote sensing for quantifying vehicular emissions (Davison and others, 2020), although this does demonstrate the capability of such methods for monitoring known sources.

Does the method need more explanation or guidance to ensure it is 'fit for purpose'?

These monitoring systems need to be used by specialists, and commonly expertise is required to ensure correct interpretation of measured concentrations. However, systems can be installed that automatically generate accessible data, for example, Swansea Council has 2 DOAS traffic monitors in place recording NO, NO_2, O_3 and benzene concentrations (City and County of Swansea, 2023). Since the approximate location of the traffic-induced concentrations is known, these systems have been installed using a fixed path from the ‘transmitter’ to the ‘receiver’. It is not, however, straightforward to predict the location of an elevated release plume, which makes application of remote sensing for industrial sources more complicated.

Limitations

Since spectroscopic techniques rely on the presence of molecular vibrations occurring at specific wavelengths, only a subset of pollutants, including O_3 and methane can be detected in the IR range. The range of pollutants with molecular vibrations occurring in the UV range is greater, and includes NO_2, SO_2 and aerosols.

In terms of the passive techniques, solar pointing methods are limited in their application to specific meteorological conditions, that is clear skies. The methods measuring scattered light generally have lower sensitivity, but are less dependent on conditions, and some configurations can provide spatial information.

Some active remote sensing systems are complex and expensive, for example, National Physical Laboratory’s DIAL. Consequently, DIAL is used in applications where detailed range-resolved emission measurements are required, rather than in long-term air quality assessments.

There are also only a small number of DIAL systems operating using IR capability available across the world. For example, beyond National Physical Laboratory’s system, there are only 2 other DIAL systems available, both of which are located in Asia. While there are a number of other DIAL systems that work in the UV range, there are currently no mobile systems operational in the UK.

Possible improvements

The majority of the systems mentioned have ongoing development, and as the technologies advance, system accessibility becomes more widespread. This has been seen in the application of remote sensing to the detection of vehicle emissions, which is now commonplace.

A4.17 Siting of monitors and network optimisation

The siting of air quality monitors is dependent on the purpose of the network. For example, in order to monitor for compliance, locations must meet criteria set out within Annex III of the Air Quality Directive (The European Parliament and the Council of the European Union, 2008), while monitoring to understand spatial patterns will require coordination with meteorology and position relative to a source. Main drivers for the siting of monitors commonly include levels of population exposure and proximity to ecosystems.

Does the method need more explanation or guidance to ensure it is 'fit for purpose'?

There are a number of guidance documents to help the selection process, including:

- Annexes III to VI and VIII of the Air Quality Directive (The European Parliament and the Council of the European Union, 2008)
- Local Air Quality Management: Technical Guidance 2022 (Defra, 2022)
- ‘Sampling points for air quality’, prepared by the European Parliament (Nagl and others, 2019)
- ‘Guide for monitoring air quality in London’ prepared by the Greater London Authority (Greater London Authority, 2018)
- ‘A Guide for Local Authorities Purchasing Air Quality Monitoring Equipment’ prepared by AEA Technology plc for Defra and the devolved administrations (Mooney, 2006)

Increasing the availability and resolution of data by installing additional monitors in areas previously unmonitored, could, however, present an issue to the Environment Agency and other regulatory bodies if the additional monitoring uncovers air quality problems that were previously unknown. In that situation, guidance would be necessary to enable regulators to respond in a coordinated manner.

Limitations

The spatial distribution of national monitors across the UK is available online (Defra, 2023f). By way of an example, Figure A4.7 shows the current siting of Automatic Urban and Rural Network (AURN) monitors (left) and the UK Eutrophying and Acidifying Pollutants (UKEAP) network of ammonia monitors (right) across the UK (Defra, 2023f). There are 2 main observations, with similar general trends in spatial configuration also evident in a number of the other national networks:

- A considerable number of air quality monitors are located at roadside locations (for the AURN) and urban background locations (for UKEAP). There is an absence of monitors located in coastal areas, which limits the understanding of shipping emissions. This could be particularly important if ammonia as a fuel gains traction in the maritime industry, from both a combustion products perspective (for associated NOx emissions) and accidental releases purposes (spillage of ammonia in transit).

- There are comparably fewer monitors in the north-west of England and west Wales; this is a feature replicated in many other national networks, including the black carbon, non-aromatic hydrocarbon and UK urban NO_2 networks, and which is an artefact of the focus of the Air Quality Directive to site monitors in densely populated areas.

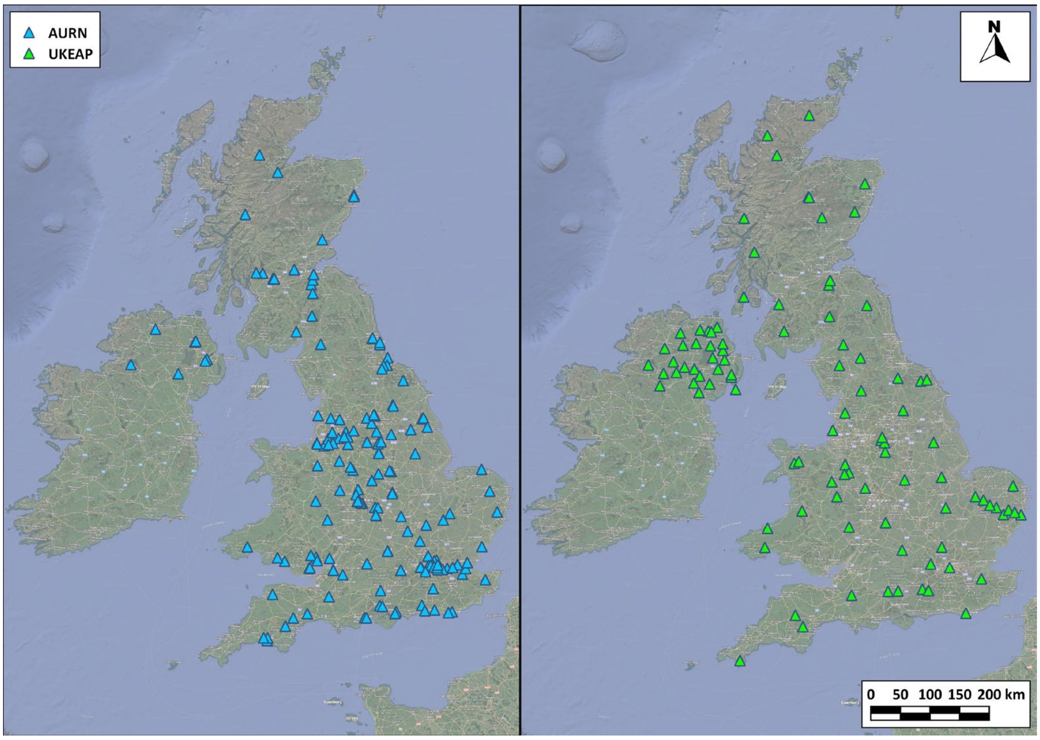


Figure A4.7: Distribution of AURN monitors (left) and UKEAP network of ammonia monitors (right) Across the UK (Defra, 2023f). Imagery ©2023 TerraMetrics, Map data ©2023 Google, GeoBasis-DE/BKG (©2009)

An Air Quality Expert Group (AQEG) report (2015) also identified that there is a lack of co-located and/or suitable reference weather data, recommending that meteorological measurements were incorporated into a number of main sites.

Possible improvements

The use of mobile monitoring can be a useful reconnaissance process to determine where to locate static sites in order to maximise the value of the network (for example, to know where to measure the highest concentrations), since intensive monitoring over a large geographical area can be carried out. Alternatively, models spanning a large geographical area can be useful to pinpoint areas where static sites should be positioned.

The current approach to the siting of national monitors is principally led by the requirement to measure compliance with the Air Quality Directive (The European Parliament and the Council of the European Union, 2008) and the specific sources of pollution set against the limit values. This approach generally leads to a balanced distribution of monitors in roadside, urban background and rural locations. It is, however, understood that the AURN is in the process of responding to the $PM_{2.5}$ requirements set out in the Environment Act (2021) with respect to monitoring in urban background and 'near source' locations. The ozone monitoring network is also currently being enhanced to cover rural areas. Therefore, while the AURN has traditionally focused on populated areas and road emissions sources, it continues to respond to emerging areas of concern, which are shifting to also include urban background and rural areas. Similarly, the location of monitors may need to adapt according to emerging technologies, which may lead to different distributions of existing pollutants, particularly those that undergo rapid transformation processes in the atmosphere.

To align with the government's social agenda, the siting of $PM_{2.5}$ monitors in the future should consider indices of multiple deprivation and population size. Studies have demonstrated that a higher proportion of people from non-white ethnic backgrounds and communities with higher levels of deprivation are more likely to be exposed to poorer air quality (Williamson and others, 2021).

The use of multiple-criteria decision analysis (MCDA) may optimise the site selection process, by enabling decisions to be made based on comparisons of different options (Kimbrough and Vallero, 2009). Options that do not meet certain criteria set by the user are gradually removed, leaving options for which interdependencies can be identified, sorted and prioritised. The MCDA process then leads to the optimum selection that meets the set of decision criteria. It should, however, be borne in mind that the requirements to meet the macro- and micro-siting criteria for compliance monitoring, as defined in the Air Quality Directive, will continue to apply, and may not be satisfied by using MCDA.

Uncertainty

As part of the quality assurance/quality control requirements set out in the Air Quality Directive, each monitoring station is required to have an uncertainty budget calculation completed.

The uncertainty associated with the monitoring network will be a product of the instrument deployed, the calibration gases used, the service, maintenance and calibration procedures, the source of instrument consumables, and the pollutant being considered.

A4.18 Hierarchical networks

The principle is that there are a number of monitors with potentially lower accuracy forming a dense web across a city, feeding into a smaller number of higher accuracy monitors as you ascend the chain, culminating in a monitor, or group of monitors, with the highest accuracy and resolution. While the number of monitors may taper, the accuracy increases. The dense, lower accuracy network would investigate pollutant distribution, that can then inform the development of a lower density, more accurate network for legislative or compliance purposes. Figure A4.8 describes a hierarchical network of air quality monitors that may be used within a city.

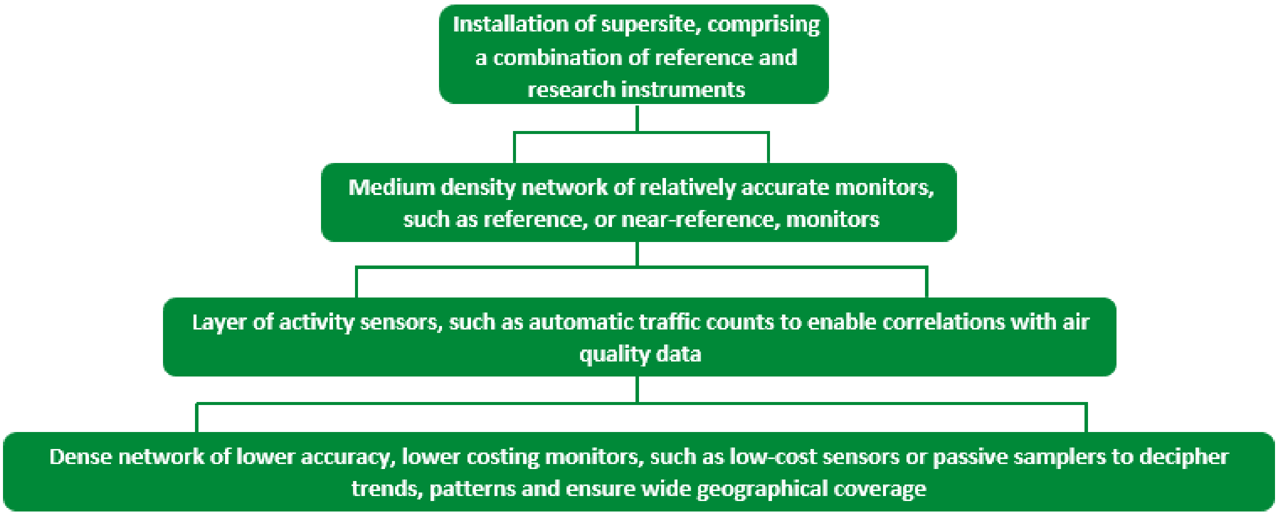


Figure A4.8: Example of hierarchical network.

The dense web of lower accuracy monitors enables the operative to have greater geographical coverage and help with selecting locations for more costly, higher value equipment. A greater geographical coverage also reduces social inequality, as lower cost methods may be used across all parts of a city, with more expensive methods targeted in ‘hot-spot’ locations. Tiers of the hierarchical network could also be coordinated with activity data, such as automatic traffic counts, to enable correlations to be determined.

From a regulatory perspective, hierarchical networks could also be used across installations, as discussed in section 2, or in response to pollution incidents. Such an approach would involve monitoring continuously using low-cost sensors (LCS) or passive samplers to determine baseline conditions at the site. If defined trigger levels were breached, more sophisticated monitoring devices with greater accuracy or smaller confidence intervals could be used. Similarly, monitoring devices with higher temporal resolutions could be used to provide greater insight and enable correlation with particular activities or meteorological conditions.

While not formally described as ‘hierarchical networks’, tiers are regularly used to coordinate the approach to monitoring air quality within the UK under the Local Air Quality Management (LAQM) requirements set out in the 1995 Environment Act (HMSO, 1995). Local authorities are mandated to carry out regular reviews and assessments of air quality in their area. Typically, this involves the use of passive samplers, such as diffusion tubes, and automatic monitors, as detailed within Defra’s Technical Guidance TG22 (Defra, 2022). Several local authorities, such as the London Borough of Lewisham and South Tyneside Council have recently been awarded funding to purchase LCS to complement their existing monitoring networks (Defra, 2023g). Oxford City Council recently installed a temporary network of low-cost air quality sensors to determine whether they could be used to improve the local evidence base and support decision making in air quality policy (OxAir, 2021).

The Breathe London scheme (Breathe London, 2023) is a further example of a hybrid monitoring network, combining reference-grade analysers alongside citizen and community-led sensor monitoring. The sensor network comprises a number of Clarity devices measuring NO_2 and $PM_{2.5}$, which, prior to deployment, are co-located with Londonair reference standard monitors. Once deployed, sensors permanently co-located with reference monitors enable real-time correction factors to be calculated, providing constant reviews of the data.

The RI-URBANS project (European Commission, 2021b), funded by the EU's Horizon 2020 programme, is seeking to reinforce cooperation between research infrastructures, such as those responsible for supersites, and monitoring networks, including promoting a higher involvement in citizen science activities.

Does the method need more explanation or guidance to ensure it is 'fit for purpose'?

Guidance is currently available in Defra's Technical Guidance TG22 (Defra, 2022) that explains how different monitor types should be used and implemented to ensure the optimum functionality. Guidance is also available that outlines how to maximise the use of monitoring and activity data from different sources to ensure effective action planning. It should, however, be noted that the term 'hierarchical' is rarely used to describe the monitoring networks.

Limitations

In order for a hierarchical network to be successfully implemented, it requires effective communication between each of the tiers. This does not, however, imply that each tier needs to be delivered by the same operator, although this would have its benefits. For instance, there may be citizen science projects with low-cost sensors ongoing in certain areas of a city, such as for academic research purposes, but the results from these are not necessarily accounted for within local authority diffusion tube networks, and their existence may not be acknowledged. For regulatory purposes, there needs to be available resource to review the data and deploy additional monitoring devices accordingly.

As such, a major limitation to current hierarchical networks is the absence of online database infrastructure that records information in a concise and standardised manner and enables users to review available data. There also needs to be confidence in the data submitted as part of any database, which is partly related to assurances surrounding the monitoring instruments used, as well as the monitoring strategy.

Possible improvements

Developing a platform for sharing and combining data from separate sources is integral to the successful delivery of a hierarchical network, as are the data assimilation methods used. While there may be confidentiality and privacy issues to overcome (assuming different operators are responsible for different tiers), it is likely that certain details could be withheld to enable at least a database of locations to be freely and openly available.

Where LCS are deployed as part of a hierarchical network, methods for cross-network calibration will need to be investigated, which may involve periodic single site calibrations or mobile transfer standards.

Uncertainty

Theoretically, the uncertainty associated with each measurement tier reduces as the hierarchy is ascended. However, this will depend on the monitoring devices that form the hierarchy.

For instance, the network may involve the deployment of numerous capped diffusion tubes (see 'Passive samplers', section A4.11) as part of a lower tier. However, these passive samplers have been shown to meet reference equivalent standards, therefore, there may not be any variability in uncertainty across the hierarchy.

A4.19 Data assimilation

Data assimilation involves combining observed data with modelled data to enhance the performance of the model and improve the estimation of the modelled output. However, it is important that scientifically defensible approaches are applied. Data assimilation is regularly used in mesoscale meteorological models (such as in numerical weather prediction (NWP)), to improve the performance of chemical transport models (CTMs), and in the analysis of atmospheric composition (such as satellite data as part of Copernicus Atmosphere Monitoring Service (CAMS)).

Current main methods

The complexity of data assimilation methods can vary significantly, depending on the scale of adjustment applied (global, spatial or temporal):

- simple linear regression methods are typically used in road traffic air quality assessments to globally verify a dispersion model (Defra, 2022)
- geostatistical methods using kriging or weighting techniques can spatially calibrate modelled concentrations
- Bayesian assimilation methods account for uncertainties in the observed data, and under certain conditions can assimilate the data, both temporally and spatially (Sandu and Chai, 2011)

A comprehensive review of data assimilation techniques was previously prepared for the Environment Agency in 2008 (Ball and others, 2008), and, therefore, has not been repeated here.

Limitations

There is a large spatial variation in ground-level pollutant concentrations in some areas, with high near-source pollutant concentration gradients. Therefore, when using data sets for assimilation, caution must be exercised during the selection process, because the measurement selected must be representative of the domain over which it influences.

Similarly, the interpretation of any adjustment factor calculated through data assimilation of measured concentrations can be complicated where measured concentrations result from a combination of different physical processes, some of which may be non-linear.

Possible improvements

When data assimilation is used to optimise CTMs, pre-processing of the monitored satellite data is often required, since it often originates from a number of sources, which vary in availability, reliability, uncertainty and format. There are strategies in place, such as the Integrated Global Observing Strategy, to standardise databases, however these also require regular updating.

Uncertainty

Data assimilation is a valid method for improving agreement between models and measurements. However, it is important that the models are configured with sufficiently accurate input data to minimise the required model adjustment. For example, regular updates of emission inventories used as input to models should be made, rather than using adjustment factors to 'correct’ model output.

The purpose of data assimilation is to minimise uncertainty. However, this does not account for the uncertainty associated with the input data. For example, if incorrect or missing sources of emission inventories have been used in the model, this will affect the data assimilation process. Equally, if the measurement data carry a high level of uncertainty, or are not representative of the relevant modelled grid, this can distort the data assimilation process.

Models are also used to predict concentrations at a specified location, for a specific point in time, or in a certain scenario, for which monitoring data are not available. This introduces uncertainty, since there is never a complete understanding of emissions, transport of emissions or chemistry, therefore, assimilating the data can lead to incorrect corrections. Data assimilation also relies on the assumption that model biases can be extrapolated to, and continue to apply in, future scenarios and moments in time, or different locations, which is not always the case.

A4.20 Machine learning/deep learning

Machine learning (ML) is a branch of artificial intelligence (AI) that uses computer systems to analyse data and develop algorithms to improve the performance of a task. Through the use of statistical methods, algorithms are ‘trained’ to make classifications or predictions. Deep learning (DL) is a subset of ML, which uses neural networks with multiple layers to simulate the human brain, allowing the computer to ‘learn’ from large data sets. ML and DL differ by the degree of human intervention required to learn.

ML/DL are used in a number of applications, including speech recognition, entertainment recommendation engines, fraud detection, clinical research and autonomous driving.

To generate a model, ML/DL requires continuous data to be divided into 3 parts:

1. The ‘training set’, which is the sample of data used to teach the model. The model learns from these data using a supervised learning method.
2. The ‘validation set’, which is used to evaluate the performance of the model. The model parameters can then be revised to improve the model, however the data are never used for training purposes.
3. The ‘test set’, which is used to evaluate the final model, and includes carefully sampled data that encompasses a range of situations the model would typically be exposed to.

Current main methods

A number of ML/DL algorithms have been applied to the field of air quality for both forecasting purposes and retrospective data analyses, including:

- decision tree-based ensemble models: ‘decision trees’ are a supervised ML technique which make predictions based on the responses to a previous set of questions. The decision trees are often run multiple times to create an ensemble and the average outcome/result taken. This usually results in a better predictive performance of the model than relying on a single decision tree
- random forest models: a type of decision tree ensemble, whereby a random subset of data (such as measured pollutant concentrations) and a random subset of features (such as wind direction, wind speed, or temperature) are used to train the model
- artificial neural networks (ANN): these comprise layers of nodes that mimic the nerve cells in the human brain. An ANN with more than 3 layers of nodes can be considered ‘deep’. Each node can be thought of as its own linear regression model, comprising input variables, weights, a threshold and an output
- recurrent neural networks (RNN): these are a type of ANN which use sequential or time series data. They are unique due to their ‘memory’ of previous inputs to influence the current inputs and outputs. The outputs of a RNN are, therefore, dependent on previous elements in the sequence
- long short-term memory (LSTM) networks: these are a type of RNN, designed to resolve situations where traditional RNN algorithms stop learning. LSTMs seek to resolve the issue of long-term dependences by having ‘cells’ in the hidden layers of the neural network that can be programmed to exclude certain information

Examples of ML/DL documented in the literature for the field of air quality are presented below:

1. The effect of Covid-19 lockdowns across the UK was quantified, based on data sets between 2017 and 2020 (Air Quality Expert Group, 2020). Studies used boosted-

regression tree models to predict counterfactual concentrations in ‘business as usual’ case studies, assuming normal meteorology, as well as an approach that used ML to correct a global forecasting model and explain sub-grid scale measurements. The effect of Covid restrictions were then quantified based on the differences in measured and predicted concentrations.

2. Researchers in India used 5 different ML models to predict the air quality index across 23 Indian cities based on 6 years of monitoring data (Kumar and Pande, 2022). The study used metrics such as root mean square error (RMSE) and coefficients of variation (R^2) to evaluate the performance of each model.
3. A 2022 study (Gladkova and Saychenko, 2022) used ML to predict future trends in $PM_{2.5}$ concentrations for a 12-week period across 7 cities in Russia, and in doing so, determine the optimum ML method for the task. The study concluded that the LSTM networks performed the best, and most accurately reflected the change in $PM_{2.5}$ trends.
4. A study in 2021 (Alahamade and others, 2021) ‘imputed’ missing pollutant data based on multivariate time series clustering algorithms, with the aim of developing a model that could eventually reduce uncertainty in air quality assessments by back-filling missing data which arises during periods of instrument downtime. The study used data collected between 2015 and 2017 from a number of Automatic Urban and Rural Network (AURN) stations to train the algorithm, before imputing the data onto the 2018 data to assess the performance.
5. Trends in directly emitted NO_2 concentrations were estimated using data from 61 urban areas across Europe between 1990 and 2015 (Grange and others, 2017). The study used meteorological normalisation, based on the random forest ML algorithm, to evaluate over 100 million hourly measurements and identify trends in the ratios between NO_2 and NOx.
6. Google purchased BreezoMeter in 2022 (Google, 2022), which combines the use of data from a range of sources, including public and private sensor networks, satellite data and transport networks, with ML algorithms and dispersion models to predict air pollution concentrations, pollen counts and products of fires. The information is then disseminated to consumers through mobile apps, home smart devices and vehicle devices.
7. Researchers in Germany used a ML approach to derive pollutant concentrations at surface level from satellite observations (Chan and others, 2021). The study compared surface pollutant concentrations derived from the ML model and a conventional regional chemistry transport model against surface in situ measurements. The ML model was generally shown to agree more closely with the surface measurements. The researchers used the derived surface pollutant concentration maps for exposure estimates and to gauge Covid-19 pandemic impacts on air quality.

Does the technique need more explanation or guidance to ensure it is 'fit for purpose'?

An online search reveals that there are several available resources, such as webinars, websites and courses that provide guidance on the applications of AI and ML/DL, as well as how to collect and prepare training set data, choosing the type of model and the steps necessary to carry out the training process. However, identifying the most useful resources would help the air quality community apply techniques in a defensible manner, although such documents would require regular updates to ensure alignment with the latest developments in the ML/DL field. Several platforms, such as GitHub (2023) and OpenAir (Carslaw and Ropkins, 2012) also offer open sources of code suitable for the analysis of air quality data. However, the development of the model and a judgement of suitability in the end result will ultimately lie with the user.

Comparisons between the measured test data and predicted results, using suitable statistical analysis methods, will identify whether the training has been successful, and guidance relating to the evaluation of significance should be prepared to provide a framework for users to use as part of the final evaluation process.

Limitations

While the application of ML/DL is a powerful tool, there are circumstances where the application of simpler statistical techniques could yield the same outcome. ML/DL also cannot truly be used as a diagnostic tool, since, while it can forecast and predict the effect of a variable, it is unable to describe the mechanism that leads to any calculated effect. As a result, ML/DL can sometimes be viewed as a ‘black box’, leading to complexities explaining the technique to non-specialists and difficulties establishing whether the outputs have been arrived at by chance and coincidental matching or through correct forecasting and prediction. Results of sensitivity testing that demonstrate a system’s ability to replicate physical processes should, therefore, accompany any ML/DL application to air quality assessments.

Suitable training of models requires a substantially sized, high quality data set. The presence of outliers and missing data in the training sets can understandably affect the training process. Similarly, data sets constrained by limited volumes of data can affect the performance of the end model, while teaching a model to predict concentrations into the future relies on an understanding of trends in concentrations for several preceding years from which it can learn.

Depending on the size of the data sets used in the model, ML/DL can be resource-consuming, and can require high-performance-computing-powered mainframes. Similarly, the need for computational power can lead to increased operational costs, such as the requirement to purchase suitable technological equipment to manage the size of the training data sets (Chen and others, 2020).

ML/DL models function better when the data used for the training, validation and test stages exhibit a normal distribution (that is, when they cover a wide range of concentrations), rather than exhibiting any type of skew (in other words, only covering a small range of concentrations). Using skewed data sets in ML/DL models can lead to underperformance, violations of model assumptions or impair the interpretation of certain features. To address skewed variables, data sets need to be manipulated using transformations (such as square root, reciprocal or log transformations) to renormalise the distribution and prepare the data set.

To meet the minimum data requirements, data sets used within ML/DL models may not all originate from the same source, and, therefore, may have different spatial and temporal resolutions. It is, therefore, necessary to pre-process the data to homogenise these resolutions, so that the data can be used in the model training stage.

Possible improvements

In order to meet the minimum data requirements (time periods, environments, pollutants) to suitably train ML/DL models, substantial quantities of air quality data are required. The requirement for data volume may be met by using dense networks of low-cost sensors. However, improvements in the way data are managed (in terms of making it freely available and in a consistent format) and better constrained uncertainty information is necessary.

Ultimately, to benefit fully from ML/DL methods, as much data as possible is needed, which may require further developments into online sharing platforms to ensure the security of the data.

Uncertainty

ML/DL is typically applied when there are no representative measurement data, and, therefore, is predicated on the assumption that trends can be extrapolated to different situations, locations and time periods. While ML/DL may provide an answer, as with any predictive tool, caution needs to be exercised to ensure that the weight given to the outcome reflects the degree of estimation inherent to the integration process.

Standard performance parameters, such as RMSE and the coefficient of determination (R^2) are used to assess the performance of the model. These parameters vary depending on the choice of model and the quality of the data used to train the model.

A4.21 Satellite measurements

Satellite measurements at short wavelengths detect solar backscattered radiation from the Earth’s surface and atmosphere. For NO_2 and several other trace gases (for example, formaldehyde, CO and methane) along with water vapour, this allows the total column between ground-level and the satellite to be determined. For ozone, height-resolved distributions are retrieved which resolve a lower tropospheric layer. Satellite measurements at IR wavelengths measure thermal emission from the Earth's surface and atmosphere during both day and night. Their vertical sensitivity to atmospheric trace gases depends on temperature contrast with the surface and typically peaks in the free troposphere, although extends to the surface in the presence of air-ground temperature contrast. At IR wavelengths, column amounts of additional trace gases can be retrieved (for example, volatile organic compounds (VOCs) such as ammonia, isoprene and methanol) and height-resolved distributions of ozone, CO, methane and water vapour can be retrieved. Satellite measurements of aerosol are principally made using backscattered solar radiation at short wavelengths, and primarily determine aerosol optical depth in the atmospheric column. Depending on spectral coverage, resolution and polarisation sensitivity, additional information on particle size distribution and type can also be acquired.

Auxiliary information on the stratospheric distribution of NO_2 allows tropospheric columns to be determined from total columns. While estimates of near-surface concentrations are possible through data assimilation or other approaches using transport models and/or ML, there is a considerable degree of uncertainty.

As indicated above, current and planned satellites enable a plethora of pollutants to be measured, including NO_2, SO_2, ammonia, CO, carbon dioxide, VOCs (including methane and isoprene from vegetation), aerosols (including particulate matter, dust and smoke), ozone and water vapour. The range of pollutants available to a specific satellite type depends on the spectral signal that can be detected. Recently, commercial products from high-resolution shortwave imaging sensors (for example, GHGSat (2023)) targeted at the oil and gas, agriculture, financial services, waste and power generation industries have become available to detect methane emissions and provide insight to enable users to take action and make informed decisions. Aerial images retrieved from satellites have also been used to provide activity data inputs for modelling, including determining agricultural sources (pig farms, chicken sheds and slurry), to count vehicle numbers for refining city-wide emissions maps (European Space Agency, 2022), and for recording natural capital databases (such as documenting greenspace assets) (Vivid Economics, 2022).

Information from satellites has a wide range of applications and advantages:

- Pollutant concentrations can be estimated across a broad geographical area, ranging from specific sources up to continental resolution for geostationary satellites to global coverage for polar orbit satellites.
- Satellite data can be used to estimate concentrations in areas in between those covered by ground-level networks (and incoming plumes overseas surrounding the UK).
- Since satellites measure concentrations in a column, rather than at surface-level, they have applications in monitoring studies of plume dispersion.
- Data can be used to identify regional sources of pollution that may affect air quality, and can be compared to regional models.

- Data can be used to establish temporal trends in yearly data, for example, using ozone and aerosol observations which date back to 1995 or trace gases which date back to 2007.
- Data can be useful for verifying emissions inventories, particularly for greenhouse gas emissions or emissions from larger sources (such as large power plant).
- The imagery enables visualisation of incoming plumes, such as from natural disasters (for instance, wildfires, or the Nord Stream pipeline explosion).

The spatial and temporal resolution depends on the satellite involved, and, as technological advances are made, these parameters are improving; a selection of satellites include:

- the Sentinel-5 Precursor satellite, which was launched in 2017 by the European Space Agency (ESA) and measures atmospheric trace gases, aerosols and cloud distribution. The satellite is in polar orbit, measuring global coverage daily at a spatial resolution as high as 7km x 3.5km (European Space Agency, 2023)
- the Geostationary Environment Monitoring Spectrometer (GEMS), which was launched in 2020 by the Korean Aerospace Research Institute, and measures columns of atmospheric ozone, NO_2, SO_2, formaldehyde and glyoxal. The satellite represents one of the new generation satellites on a geostationary platform, enabling it to capture the diurnal variation of pollutants in the troposphere and stratosphere. The satellite records at an hourly resolution (30 minutes imaging, 30 minutes rest) from a geostationary orbit covering Asia with a spatial resolution spanning 4 x 8km (Atmospheric Radiation Laboratory, 2023)
- the Metop-A/B/C satellites, the first of which was first launched in 2007 by the ESA, and which has both shortwave and IR spectrometers to measure concentrations of ozone, NO_2, and SO_2, ammonia, CO, methanol and methane alongside data relating to humidity and temperature. The satellite is in a sun-synchronous polar orbit, providing global observations twice daily (in the IR), with resolutions ranging between 12km and 50km, depending on the instrument (World Meteorological Organisation, 2023)
- next generation operational satellites include MTG-I and MTG-S to observe from a geostationary orbit over UK and Europe and to provide hourly coverage of trace gases and particulates as well as MetOp-SG in polar orbit to provide higher quality data than MetOp through to the 2040s

A review of satellite monitoring in the context of the Environment Agency’s regulatory responsibilities was carried out in 2021 (Brown and others, 2021). The purpose of the review was to identify whether satellite data were of value to the Environment Agency, and to develop analysis techniques to enable satellites to help the Environment Agency fulfil its regulatory responsibilities.

Does the technique need more explanation or guidance to ensure it is 'fit for purpose'?

The satellites are operated by international and national space agencies, such as ESA and NASA; however, data are publicly available online. It is, therefore, important that the raw satellite data are appropriately processed for use. Raw satellite data are required to undergo 3 stages of processing before they are fit for use in any air quality application:

- The raw data are transformed from ‘counts’ to recognised ‘radiance units’, and linked to geospatial information such as latitude, longitude, date and time. The data are calibrated spectrally and radiometrically, and adjusted for bias, to produce L1 data.
- Distributions of geophysical variables, including trace gases and aerosol are then ‘retrieved’ from radiance spectra using ‘inverse methods’ to produce L2 data.
- Depending on application, data can be ‘regridded’, and/or averaged spatially or temporally, or grouped to produce L3 data, according to condition to enable them to be used.

Carrying out these steps requires expert knowledge and skills, since they include the use of assumptions and priori information to constrain the analysis, therefore, detailed guidance is needed if they were to become widely used within the air quality community. It may also be possible, during the early stages of satellite product development, to incorporate the needs and requirements of the air quality community, to ensure that the full benefits are harnessed.

Limitations

With some exceptions (ozone and IR measurements of CO, methane and water vapour), satellite sensors provide column abundances and do not resolve vertical layers. Developments are, however, in progress to exploit co-located shortwave and IR observations to resolve lower tropospheric concentrations. In order to estimate near-surface concentrations, auxiliary information is required on vertical profile shape, for example from CTMs, or else data assimilation or ML methods have to be used, together with a number of assumptions, which introduces an additional layer of uncertainty to the measurements.

As described above, a number of satellites are operating in polar sun-synchronous orbit. As a result, trace gas data are currently captured on a daily or twice daily basis, resulting in reduced temporal resolutions. On the other hand, geostationary satellites provide observations approximately every hour. The Meteostat Second Generation satellite provides this for aerosol, as MTG-I will do so too. GEMS provides observations over south-east Asia for trace gases observable in the shortwave region. The Tropospheric Emissions: Monitoring of Pollution (TEMPO) satellite, which has just been launched by NASA, will provide observations over the United States. MTG-S will do this for both shortwave and IR over Europe. Cloud cover obscures the atmosphere below; since cloud cover is generally greater during winter, calculations of annual averages may be biased by summertime measurements when there is greater availability of measurement data.

Satellite instruments have a wide spatial coverage, and while the actual spatial resolution of the instruments is improving, it still remains limited, with each concentration datapoint returned from a satellite covering several kilometres.

Information relating to a number of chemical species may be planned for a satellite mission. However, onboard instruments may fail, or the satellite may encounter difficulties such as collisions and inclement weather. It is, therefore, commonplace for multiple satellites to be deployed.

Possible improvements

The Sentinel EO-based Emissions and Deposition Service (SEEDS) project is linked to the future evolution of the Copernicus Atmosphere Monitoring Service (CAMS) and aims to develop several satellite inversion techniques to estimate European emissions of NOx, ammonia, VOC, improve deposition flux modelling, and develop advanced data assimilation techniques. The project is developing techniques that may eventually become part of the CAMS. The project is now entering its third and final year and a significant number of data sets have been compiled for further evaluation (SEEDS, 2023).

Four improved satellites, specifically planned for measuring a range of pollutants (gases such as NO_2, ozone, SO_2 and formaldehyde, as well as aerosols), have either recently been launched, or are scheduled to launch over the next few years:

- MTG-I with a Flexible Combined Vis/IR Imager has been launched and will observe at 1 x1km resolution at 10-minute intervals in the shortwave.
- The TEMPO satellite has just been launched by NASA. The satellite will record at an hourly resolution from a geostationary orbit covering an area of North America with a spatial resolution spanning 2 x 5km.
- The geostationary MTG-S satellite will be launched in 2024 by Eumetsat and will measure air quality across Europe and Northern Africa. The Sentinel 4 shortwave instrument (part of the Copernicus programme) will have a revisit time of 60 minutes, and a spatial resolution of 8 x 8km^2. The Infrared Sounder (IRS) will have a shorter revisit time and spatial resolution of 4 x 4km^2.
- MetOp-SG is due to be launched in 2025 by Eumetsat with sensors operating in the shortwave (Sentinel-5) and IR (IASI-NG) with advanced capabilities on MetOp along with the vis/IR imager MetImage and polarimeter 3MI for aerosol.

The improved satellites, alongside the GEMS instrument, will form a global constellation of satellites, capable of measuring air quality at hourly resolution. These, along with MetOp-SG and subsequently CO2M, are anticipated to revolutionise the monitoring of atmospheric pollutants over the Northern Hemisphere.

Uncertainty

Satellite data may be subject to errors arising from sensor drift, sensor calibration, bias in algorithm parameters used to analyse the data, and choice of priori constraints. The conversion of satellite observations into useable concentration data also relies on deterministic models and current, reliable, emissions inventories, the quality of which may vary. The level of uncertainty associated with individual satellite measurements at particular locations is, therefore, difficult to quantify conclusively. However, it is likely to be greater than the uncertainty associated with in-situ monitors (Vijayaraghavan and others, 2008).

Nonetheless, the value of satellite observations rests in their complementary attributes, including their spatial density, vertical extent and multi-decade continuity.

References

ADMS-Puff (2023), [Online], Available: https://www.cerc.co.uk/environmental-software/ADMS-Puff-model.html [Sep 2023].

ADMS-STAR (2023), [Online], Available: https://www.cerc.co.uk/environmental-software/ADMS-STAR-model.html [Sep 2023].

Aeroqual (2021) *Case Studies: Compact Monitoring System Facilitates Mobile Air Quality Study on Major European Highways*, [Online], Available: https://aeroqual.imgix.net/assets/documents/Egnatia_Odos_Motorway_Case_Study_2021-11-16-064309_loso.pdf [Sep 2023].

Aether (2023) 'Emissions from Hydrogen Combustion and NH3 as a Fuel in the Marine Sector'.

Air Quality Consultants Ltd (2018) 'Ashdown Forest SAC: Air Quality Monitoring and Modelling - Volume 1'.

Air Quality Expert Group (2005) 'Particulate Matter in the United Kingdom: Chapter 5 - Methods for Monitoring Particulate Concentrations'.

Air Quality Expert Group (2015) 'Evidential Value of Defra Air Quality Compliance Monitoring'.

Air Quality Expert Group (2020) 'Estimation of Changes in Air Pollution Emissions, Concentrations and Exposure during the Covid-19 Outbreak in the UK'.

Alahamade, W., Lake, I., Reeves, C.E. and De La Iglesia, B. (2021) 'Evaluation of multivariate time series clustering for imputation of air pollution data', *Geoscientific Instrumentation Methods and Data Systems*, vol. 10, pp. 265–285, Available: https://gi.copernicus.org/articles/10/265/2021/gi-10-265-2021.pdf.

Allan, J., Harrison, R. and Maggs, R. (2022) *Measurement Uncertainty for PM2.5 in the Context of the UK National Network*, Defra.

Almbauer, R.A., Ottl, D., Bacher, M. and Sturm, P.J. (2000) 'Simulation of the air quality during a field study for the city of Graz', *Atmospheric Environment*, vol. 34, no. 27, pp. 4581 - 4594.

ANSYS (2023) *Products*, [Online], Available: https://www.ansys.com/en-gb/products/fluids/ansys-fluent [Sep 2023].

AQTAG (2011) *AQTAG06 - Technical guidance on detailed modelling approach for an appropriate assessment for emissions to air*.

Atmospheric Measurement and Observation Facility (2023) *Mobile Air Quality Supersites*, [Online], Available: https://amof.ac.uk/observatory/community-observatory-mobile-air-quality-supersites/ [Sep 2023].

Atmospheric Radiation Laboratory (2023) *GEMS Instrument*, [Online], Available: http://gems1.yonsei.ac.kr/sub01/sub02.php [Sep 2023].

Ball, A., Hill, R. and Jenkinson, P. (2008) 'Integration of air quality modelling and monitoring methods: review and applications' Environment Agency, Available: https://assets.publishing.service.gov.uk/government/uploads/system/uploads/attachment_data/file/290553/scho0308boae-e-e.pdf.

Benavides, J., Snyder, M., Guevara, M., Soret, A., Pérez García-Pando, C., Amato, F., Querol, X. and Jorba, O. (2019) 'CALIOPE-Urban v1. 0: coupling R-LINE with a mesoscale air quality modelling system for urban air quality forecasts over Barcelona city (Spain)', *Geoscientific Model Development*, vol. 12, pp. 2811-2835.

Berkowicz, R., Olesen, H.R. and Torp, U. (1986) 'The Danish Gaussian air pollution model (OML): Description, test and sensitivity analysis in view of regulatory applications' Springer US.

Bowman, K.P., Lin, J.C., Stohl, A., Draxler, R., Konopka, P., Andrews, A. and Brunner, D. (2013) 'Input data requirements for Lagrangian trajectory models', *Bulletin of the American Meteorological Society*, vol. 94, no. 7, pp. 1051 - 1058.

Bowyer, T.W., Kephart, R., Eslinger, P.W., Friese, J.I., Miley, H.S. and Saey, P.R.J. (2013) 'Maximum reasonable radioxenon releases from medical isotope production facilities and their effect on monitoring nuclear explosions', *Journal of Environmental Radioactivity*, vol. 115, pp. 192 - 200.

Breathe London (2023) *Breathe London: The Community Sensing Network*, [Online], Available: https://www.breathelondon.org/about [Sep 2023].

Brown, A., Hayward, T., Timmis, R., Wade, K., Pope, R., Trent, t., Boesch, H. and Barrio Guillo, R. (2021) 'Satellite measurements of air quality and greenhouse gases: application to regulatory activities' Environment Agency, Available: https://assets.publishing.service.gov.uk/government/uploads/system/uploads/attachment_data/file/983740/Satellite_measurements_of_air_quality_and_greenhouse_gases_-_report.pdf.

Butterfield, D., Martin, N.A., Coppin, G. and Fryer, D.E. (2021) 'Equivalence of UK nitrogen dioxide diffusion tube data to the EU reference method', *Atmospheric Environment*, pp. 262, 118614.

Byun, D. and Schere, K.L. (2006) 'Components of the Models-3 Community Multiscale Air Quality (CMAQ) Modeling System', *Applied Mechanics Reviews*, pp. 51 - 77.

C40 Cities (2022) 'Sensing Change: How Cities are Using New Sensing Technologies to Achieve Air Quality Goals'.

CALPUFF Modeling System (2023), [Online], Available: http://www.src.com/ [Sep 2023].

Candice Lung, S.C., Jones, R., Zellweger, C., Karppinen, A., Penza, M., Dye, T., Hüglin, C., Ning, Z., Lewis, A.C., von Schneidemesser, E., Peliter, R.E., Leigh, R., Hagan, D., Laurent, O. and Carmichael, G. (2018) 'Low-cost sensors for the measurement of atmospheric composition: overview of topic and future applications' World Meteorological Organisation.

Carpenter, D.O., Arcaro, K. and Spink, D.C. (2002) 'Understanding the Human Health Effects of Chemical Mixtures', *Environmental Health Perspectives: Reviews*, vol. 110, no. 1.

Carruthers, D.J., Holroyd, R.J., Hunt, J.C.R., Weng, W.S., Robins, A.G., Apsley, D.D., Thompson, D.J. and Smith, F.B. (1994) 'UK-ADMS: A new approach to modelling dispersion in the earth's atmospheric boundary layer', *Journal of wind engineering and industrial aerodynamics*, vol. 52, pp. 139-153.

Carruthers, D.J., Hunt, J.C.R. and Weng, W.S. (1988) 'A computational model of stratified turbulent airflow over hills - FLOWSTAR I', *Proceedings of ENVIROSOFT: computer techniques in environmental studies*, pp. 481 - 492.

Carruthers, D., Stocker, J., Stidworthy, A., Hood, C., Jackson, R., McCosh, G.. and Reis, S. (2022) 'Defra 2021 Air quality Model Inter-Comparison Exercise' Aveiro, Portugal: 21st International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes 27-30 September 2022.

Carslaw, D.C. and Ropkins, K. (2012) 'OpenAir - An R Package for Air Quality Data Analysis', *Environmental Modelling and Software*, vol. 27-28, no. 52-61.

Casciaro, G., Cavaiola, M. and Mazzino, A. (2022) ' Calibrating the CAMS European multi-model air quality forecasts for regional air pollution monitoring', *Atmospheric Environment*, pp. 287, 119259.

Castell, N., Clements, A.L., Dye, T., Hüglin, C., Kroll, J.H., Candice Lung, S.C., Ning, Z., Parsons, M., Penza, M., Reisen, F. and von Schneidemesser, E. (2020) 'An Update on Low-cost Sensors for the Measurement of Atmospheric Composition' World Meteorological Organisation.

CDL Tecora (2023) *VOC Passive Sampler GABIE*, [Online], Available: https://www.tecora.com/en/produit/6415/ [Sep 2023].

Chan, K.L., Khorsandi, E., Liu, S., Baier, F. and Valks, P. (2021) 'Estimation of Surface NO2 Concentrations over Germany from TROPOMI Satellite Observations using a Machine Learning Method', *Remote Sensing*, vol. 13, no. 5, p. 969.

Chatani, S., Morikawa, T., Nakatsuka, S., Matsunaga, S. and Minoura, H. (2011) 'Development of a framework for a high-resolution, three-dimensional regional air quality simulation and its application to predicting future air quality over Japan', *Atmospheric Environment*, vol. 45, pp. 1383-1393.

Chen, C., Zhang, P., Zhang, , Dai, , Yi, Y., Zhang, and Zhang, Y. (2020) 'Deep Learning on Computational-Resource-Limited Platforms: A Survey', *Mobile Information Systems*, vol. 2020, Available: Article ID 8454327.

Chowdhury, B., Karamchandani, P.K., Sykes, R.I., Henn, D.S. and Knipping, E. (2015) 'Reactive puff model SCICHEM: Model enhancements and performance studies', *Atmospheric Environment*, vol. 117, pp. 242-258.

Cimorelli, A.J., Perry, S.G., Venkatram, A., Weil, J.C., Paine, R.J., Wilson, R.B., Lee, R.F., Peters, W.D. and Brode, R.W. (2005) 'AERMOD: A dispersion model for industrial source applications. Part I: General model formulation and boundary layer characterization', *Journal of Applied Meteorology and Climatology*, vol. 44(5), pp. 682-693.

City and County of Swansea (2023) *Online Air Quality and Meteorological Readings in Swansea*, [Online], Available: https://swansea.airqualitydata.com/ [Sep 2023].

Clappier, A., Thunis, P., Pirovano, G., Riffault, V., Gilardoni, S., Pisoni, E., Guerreiro, C., Monteiro, A., Dupont, H., Wærsted, E., Hellebust, S., Stocker, J., Eriksson, A., Angyal, A., Bonafe, G., Montanari, F., Matejovica, J., Bartzis, J. and Gianelle, V. (2022) 'Source apportionment to support air quality management practices' Publications Office of the European Union.

Clements, A.R., Duvall, D., Greene, A.N.D. and Dye, T. (2022) 'The Enhanced Air Sensor Guidebook'.

Collins, W.J., Stevenson, D.S., Johnson, C.E. and Derwent, R.G. (1997) 'Tropospheric ozone in a global-scale three-dimensional Lagrangian model and its response to NOx emission controls', *Journal of Atmospheric Chemistry*, vol. 26, pp. 223 - 274.

Committee on the Medical Effects of Air Pollutants (2023).

Cummings, L.E., Stewart, J.D., Reist, R., Shakya, K.M. and Kremer, P. (2021) 'Mobile monitoring of air pollution reveals spatial and temporal variation in an urban landscape', *Frontiers in Built Environment*, pp. 7, 648620.

Davison, J., Bernard, Y., Borken-Kleefeld, J., Farren, N.J., Hausberger, S., Sjödin, Å., Tate, J.E., Vaughan, A.R. and Carslaw, D.C. (2020) 'Distance-based emission factors from vehicle emission remote sensing measurements', *Science of the Total Environment*, vol. 739, p. 139688.

Defra (2016) 'Quality Assurance and Quality Control (QA/QC) Procedures for UK Air Quality Monitoring under 2008/50/EC and 2004/107/EC'.

Defra (2018) *AQEG Advice on the Use of 'Low-cost' Pollution Sensors*, [Online], Available: https://uk-air.defra.gov.uk/research/aqeg/pollution-sensors.php [Sep 2023].

Defra (2022) *Review & Assessment: Technical Guidance LAQM.TG22 August 2022 Version*, [Online], Available: https://laqm.defra.gov.uk/wp-content/uploads/2022/08/LAQM-TG22-August-22-v1.0.pdf [Sep 2023].

Defra (2023a) 'Emissions of Air Pollutants in the UK - Ammonia (NH3)'.

Defra (2023b) 'UKEAP: National Ammonia Monitoring Network'.

Defra (2023c) 'Emissions of Air Pollutants in the UK - Nitrogen Oxides (NOx)'.

Defra (2023d) *Site Information Search*, [Online], Available: https://uk-air.defra.gov.uk/networks/search-site-info [Sep 2023].

Defra (2023e) *EU Standard Methods for monitoring and UK Approach*, [Online], Available: https://uk-air.defra.gov.uk/networks/monitoring-methods?view=eu-standards [Sep 2023].

Defra (2023f) *Interactive Monitoring Networks Maps*, [Online], Available: https://uk-air.defra.gov.uk/interactive-map [Sep 2023].

Defra (2023g) *Defra press release*, [Online], Available: https://www.gov.uk/government/news/107-million-in-funding-for-local-authorities-to-improve-air-quality [Sep 2023].

Department for Business, Energy and Industrial Strategy (2019) 'Clean Growth Grand Challenge: Industrial Clusters Mission - Infographic'.

Di Sabatino, S., Leo, L.S., Cataldo, R. and Ratti, C. (2010) 'Construction of Digital Elevation Models for a Southern European City and a Comparative Morphological Analysis with Respect to Northern European and North American Cities', *Journal of Applied Meteorology and Climatology*, vol. 49, no. 7, pp. 1377 - 1396.

Dickerson, R.R. (2015) 'The Regional Atmospheric Measurement, Modelling and Prediction Program (RAMMPP) 2015'.

Diez, S., Lacy, S.E., Bannan, T., Flynn, M., Gardiner, T., Harrison, D., Marsden, N., Martin, N.A., Read, K. and Edwards, P.M. (2022) 'Air pollution measurement errors: is your data fit for purpose?', *Atmospheric Measurement Techniques*, vol. 15, no. 13, pp. 4091 - 4105.

Douglas, P., Robertson, S., Gay, R., Hansell, A.L. and Gant, T.W. (2018) 'A systematic review of the public health risks of bioaerosols from intensive farming', *International Journal of Hygiene and Environmental Health*, vol. 221, no. 2, pp. 134 - 173.

Draxler, R.R. and Hess, G.D. (1997) 'Description of the HYSPLIT_4 modelling system', *NOAA Technical Memos - Air Resources Laboratory*, vol. 224, p. 24.

Duangsuwan, and Jamjareekulga, (2020) 'Development of Drone Real-time Air Pollution Monitoring for Mobile Smart Sensing in Areas with Poor Accessibility', *Sensors and Materials*, vol. 32, no. 2, Available: https://sensors.myu-group.co.jp/sm_pdf/SM2118.pdf.

Dyson (2022) *Introducing Dyson's next generation Air Quality backpacks on #CleanAirDay*, [Online], Available: https://www.dyson.co.uk/newsroom/insights/air-quality/air-quality-backpacks [Sep 2023].

Environment Act 2021 (2021).

Environment Agency (2011) *Technical Guidance Note. M8 Monitoring Ambient Air, Version 2*, Environment Agency.

Environment Agency (2019) 'Review of differential absorption lidar flare emission and performance data'.

Environment Agency (2023a) 'Options for air quality research: Drivers of future changes'.

Environment Agency (2023b) 'RDE048 and RDE049'.

Environment Agency (2023c) *Environmental permitting: air dispersion modelling reports*, [Online], Available: https://www.gov.uk/guidance/environmental-permitting-air-dispersion-modelling-reports#explain-meteorological-data-and-surface-characteristics [Sep 2023].

Environment Agency (2023d) *Guidance MCERTS performance standards for ambient monitoring equipment*, [Online], Available: https://www.gov.uk/government/publications/mcerts-performance-standards-for-ambient-monitoring-equipment/mcerts-performance-standards-for-ambient-monitoring-equipment [Sep 2023].

Environment Agency (2023e) *Ambient air monitoring performance standards*, [Online], Available: https://www.gov.uk/government/collections/monitoring-emissions-to-air-land-and-water-mcerts#ambient-air-monitoring-performance-standards [Sep 2023].

Environment, Food and Rural Affairs Committee (2022) 'Tree Planting: Third Report of Session 2021–22' House of Commons Committee, Available: https://publications.parliament.uk/pa/cm5802/cmselect/cmenvfru/356/report.html#:~:text=The%20UK%20Government%20has%20committed,created%20every%20year%20by%202025.

European Commission (2016) 'National Emissions Ceilings Regulations 2016/2284/EU'.

European Commission (2021a) *WG6 - Sensors and Data-fusion*, [Online], Available: https://fairmode.jrc.ec.europa.eu/activity/ct6 [Sep 2023].

European Commission (2021b) *RI-URBANS*, [Online], Available: https://riurbans.eu/project/ [Sep 2023].

European Commission Joint Research Centre (2023) *FAIRMODE*, [Online], Available: https://fairmode.jrc.ec.europa.eu/activity/ct4 [Sep 2023].

European Committee for Standardisation (CEN) (2005) 'Standard Methods for monitoring air pollutants'.

European Committee for Standardisation (CEN) (2021a) 'Air Quality - Performance Evaluation of Air Quality Sensor Systems - Part 1: Gaseous Pollutants in Ambient Air (CEN/TS 17660-1:2022)'.

European Committee for Standardisation (CEN) (2021b) *CEN Technical Committee 264 - Air Quality - Working Group 42 - Gas Sensors*, [Online], Available: https://standards.iteh.ai/catalog/tc/cen/1dcd8f4d-521f-465f-af1c-91ef3e852bab/cen-tc-264-wg-42 [Sep 2023].

European Cooperation in Science and Technology (2015) 'ES1006 - Evaluation, improvement and guidance for the use of local-scale emergency prediction and response tools for airborne hazards in built environments' COST ES1006.

European Space Agency (2022) *Monitoring Air Quality by Counting Vehicles*, [Online], Available: https://www.esa.int/ESA_Multimedia/Images/2022/06/Monitoring_air_quality_by_counting_vehicles [Sep 2023].

European Space Agency (2023) *Sentinel-5P: Facts and figures*, [Online], Available: https://www.esa.int/Applications/Observing_the_Earth/Copernicus/Sentinel-5P/Facts_and_figures [Sep 2023].

Flying drones and model aircraft (2023), [Online], Available: https://register-drones.caa.co.uk/ [Sep 2023].

Franke, J., Hellsten, A., Schlünzen, K.H. and Carissimo, B. (2007) 'Best practice guideline for the CFD simulation of flows in the urban environment-a summary', 11th Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, Cambridge.

Frazer-Nash Consultancy (2021) *Frazer-Nash digital twin supporting Atmo's innovative rail air quality demonstrator project*, [Online], Available: https://www.fnc.co.uk/discover-frazer-nash/news/frazer-nash-digital-twin-supporting-atmo-s-innovative-rail-air-quality-demonstrator-project/ [Sep 2023].

Frederickson, L.B., Sidaraviciute, R., Schmidt, J.A., Hertel, O. and Johnson, M.S. (2022) 'Are dense networks of low-cost nodes really useful for monitoring air pollution? A case study in Staffordshire', *Atmospheric Chemistry and Physics,* vol. 22, no. 21, pp. 13949 - 13965.

GEOS-Chem (2023) *GEOS-Chem 14.1.1*, [Online], Available: https://geoschem.github.io/ [Sep 2023].

GHGSAT (2023) *GHGSAT*, [Online], Available: https://www.ghgsat.com/en/ [Sep 2023].

Giordano, M.R., Malings, C., Pandis, S.N., Presto, A.A., McNeill, V.F., Westervelt, D.M., Beekmann, M. and Subramanian, R. (2021) 'From low-cost sensors to high-quality data: A summary of challenges and best practices for effectively calibrating low-cost particulate matter mass sensors', *Journal of Aerosol Science*, vol. 158, November, p. 105833.

GitHub (2023) *Topics*, [Online], Available: https://github.com/topics [Sep 2023].

Gladkova, E. and Saychenko, L. (2022) 'Applying machine learning techniques in air quality prediction', *Transportation Research Procedia*, vol. 63, pp. 1999-2006, Available: https://www.sciencedirect.com/science/article/pii/S235214652200477X.

Google (2022) *BreezoMeter: Delivering Global Environmental Information with Google Cloud*, [Online], Available: https://cloud.google.com/customers/breezometer [Sep 2023].

Gradko International (2023), [Online], Available: https://www.gradko.com/environmental/environmental-resources/technical-resources/ [Sep 2023].

Grange, S.K., Lewis, A.C., Moller, S.J. and Carslaw, D.C. (2017) 'Lower Vehicular Primary Emissions of NO2 in Europe than Assumed in Policy Projections', *Nature Geoscience*, pp. 914 - 918.

Greater London Authority (2018) 'Guide for monitoring air quality in London' London, Available: https://www.london.gov.uk/sites/default/files/air_quality_monitoring_guidance_january_2018.pdf.

Grell, G.A., Peckham, S.E., Schmitz, R., McKeen, S.A., Frost, G., Skamarock, W.C. and Eder, B. (2005) 'Fully coupled 'online' chemistry in the WRF model', *Atmospheric Environment*, vol. 39, no. 37, pp. 6957 - 6975.

Heal, M., Laxen, D. and Marner, B. (2018) 'review of biases in the measurement of ambient nitrogen dioxide (NO2) by Palmes passive diffusion tube.'.

Health and Safety Executive (2021) 'Review of Dense-gas Dispersion for Industrial Regulation and Emergency Preparedness and Response'.

Hill, R., Lutman, E. and Arnott, A. (2005) 'A Review of Atmospheric Dispersion in Complex Terrain'.

HMSO (1995) *1995 Environment Act*, [Online], Available: https://www.legislation.gov.uk/ukpga/1995/25/contents [Sep 2023].

Hood, C., MacKenzie, I., Stocker, J., Johnson, K., Carruthers, D., Vieno, M. and Doherty, R. (2018) 'Air quality simulations for London using a coupled regional-to-local modelling system', *Atmospheric Chemistry and Physics*, vol. 18, pp. 11221–11245.

Innocenti, F., Robinson, R., Gardiner, T., Finlayson, A. and Connor, A. (2017) 'Differential absorption lidar (DIAL) measurements of landfill methane emissions', *Remote Sensing*, vol. 9, no. 9, p. 953.

Janicke, U. and Janicke, L. (2002) 'Development of a model-based assessment system for machine-related immission control'.

Johansson, J.K., Mellqvist, J., Samuelsson, J., Offerle, B., Lefer, B., Rappenglück, B., Flynn, J. and Yarwood, G. (2014) 'Emission measurements of alkenes, alkanes, SO2, and NO2 from stationary sources in Southeast Texas over a 5 year period using SOF and Mobile DOAS', *Journal of Geophysical Research: Atmospheres*, vol. 119, no. 4, pp. 1973 - 1991.

Jones, A.R., Thomson, D.J., Hort, M. and Devenish, B. (2007) 'The U.K Met Office's next generation atmospheric dispersion model, NAME III', *Proceedings of the 27th NATO/CCMS International Technical Meeting on Air Pollution Modelling and its Application*, pp. 580 - 589.

Kimbrough, S. and Vallero, D. (2009) 'Air Pollution Monitoring Site Selection by Multiple Criteria Decision Analysis', in *McGraw-Hill Yearbook of Science & Technology 2009*, McGraw-Hill, Available: https://www.researchgate.net/publication/235926617_Air_Pollution_Monitoring_Site_Selection_by_Multiple_Criteria_Decision_Analysis.

Kozmar, H. (2010) 'Scale effects in wind tunnel modeling of an urban atmospheric boundary layer', *Theoretical and Applied Climatology*, vol. 100, pp. 153 - 162.

Kumar, K. and Pande, B.P. (2022) 'Air pollution prediction with machine learning: a case study of Indian cities', *International Journal of Environmental Science and Technology*, Available: https://link.springer.com/article/10.1007/s13762-022-04241-5#article-info.

Kwak, K.H., Baik, J.J., Ryu, Y.H. and Lee, S.H. (2015) 'Urban air quality simulation in a high-rise building area using a CFD model coupled with mesoscale meteorological and chemistry-transport models', *Atmospheric Environment*, vol. 100, pp. 167-177.

Lackner, M. (2007) 'Tunable diode laser absoprtion spectroscopy (TDLAS) in the process industries - a review', *Reviews in Chemical Engineering*, vol. 23, no. 2, pp. 65 - 147.

Liu, Y.S., Miao, S.G., Zhang, C.L., Cui, G.X. and Zhang, Z.S. (2012) 'Study on micro-atmospheric environment by coupling large eddy simulation with mesoscale model', *Journal of Wind Engineering and Industrial Aerodynamics*, vol. 107, pp. 106-117.

Lugon, L., Sartelet, K., Kim, Y., Vigneron, J. and Chrétien, O. (2020) 'Nonstationary modeling of NO 2, NO and NO x in Paris using the Street-in-Grid model: coupling local and regional scales with a two-way dynamic approach', *Atmospheric Chemistry and Physics*, vol. 20, pp. 7717-7740.

Macdonald, R.W., Griffiths, R.F. and Hall , D.J. (1998) 'An improved method for the estimation of surface roughness of obstacle arrays', *Atmospheric Environment*, vol. 32, no. 11, pp. 1857 - 1864.

Manders, A.M., Builtjes, P.J., Curier, L., Denier van der Gon, H.A., Hendriks, C., Jonkers, S. and Schaap, M. (2017) 'Curriculum vitae of the LOTOS-EUROS (v2.0) chemistry transport model', *Geoscientific Model Development* , vol. 10, no. 11, pp. 4145 - 4173.

Marais, E.A., Pandey, A.K., van Damme, M., Clarisse, L., Coheur, P.-F., Shephard, M.W., Cady-Pereira, K.E., Misslebrook, T., Zhu, L., Luo, G. and Yu, F. (2021) 'UK Ammonia Emissions Estimated with Satellite Observations and GEOS-Chem', *Journal of Geophysical Research: Atmospheres*, vol. 126, no. 18.

Martin, N.A., Ferracci, V., Cassidy, N., Hook, J., Battersby, R.M., di Meane, E.A.. and. Seitler, E. (2019) ' Validation of ammonia diffusive and pumped samplers in a controlled atmosphere test facility using traceable Primary Standard Gas Mixtures', *Atmospheric Environment*, pp. 199, 453-462.

Martin, N.A., Ferrachi, V., Cassidy, N. and Hoffnagle, J.A. (2016) 'The application of a cavity ring-down spectrometer to measurements of ambient ammonia using traceable primary standard gas mixtures', *Applied Physics B*, vol. 122, July, p. 219.

Martin, N.A., Helmore, J.J., White, S., Barker Snook, I.L., Parish, A. and Gates, L.S. (2014) 'Measurement of nitrogen dioxide diffusive sampling rates for Palmes diffusion tubes using a controlled atmosphere test facility (CATFAC)', *Atmospheric Environment*, vol. 94, September, pp. 529 - 537.

Mellqvist, J., Samuelsson, J., Rivera, C., Lefer, B. and Patel, M. (2007) 'Measurements of industrial emissions of VOCs, NH3, NO2 and SO2 in Texas using the Solar Occultation Flux method and mobile DOAS', in *Final Report HARC Project H, 53, pgs 2 - 69*.

Menut, L., Bessagnet, B., Briant, R., Cholakian, A., Couvidat, F., Mailler, S., Pennel, R., Siour, G., Tuccella, P., Turquety, S. and Valari, M. (2021) 'The CHIMERE v2020r1 online chemistry transport model', *Geoscientific Model Development*, vol. 14, no. 11, pp. 6781 - 6811.

Mooney, D. (2006) *A Guide for Local Authorities Purchasing Air Quality Monitoring Equipment*, Defra.

Moroni, S., Cruz Torres, F., Palomba, P., Dal Santo, U. and Colombi, C. (2022) 'Near Reference Air Quality Sensors Can Support Local Planning: A Performance Assessment in Milan, Italy', *Environmental Sciences Proceedings*, vol. 19, no. 36, July.

Nagl, C., Spangl, W. and Buxbaum, I. (2019) 'Sampling points for air quality, Study for the Committee on the Environment, Public Health and Food Safety' Luxembourg.

Nance, E. (2021) 'Monitoring Air Pollution Variability during Disasters', *Atmosphere*, pp. 12(4), 420.

National Library of Medicine (2023) *PubMed*, [Online], Available: https://pubmed.ncbi.nlm.nih.gov/ [Apr 2023].

National Oceanic and Atmospheric Administration (2017) *Fifty years ago, a historic balloon launch that changed the way we see the ozone layer*, [Online], Available: https://www.noaa.gov/news/fifty-years-ago-historic-balloon-launch-changed-way-we-see-ozone-layer [Sep 2023].

Natural Resources Wales (2019) 'Guidance Note: Modelling the Concentration and Deposition of Ammonia Emitted from Intensive Farming'.

Natural Resources Wales (2023) *How to carry out detailed modelling of ammonia emissions*, [Online], Available: https://naturalresources.wales/guidance-and-advice/business-sectors/farming/ammonia-assessments/how-to-carry-out-detailed-modelling-of-ammonia-emissions-gn-036/?lang=en [Sep 2023].

NCAR Laboratory: Mesoscale and Microscale Meteorology (2023) *Weather Research and Forecasting Model (WRF)*, [Online], Available: https://www.mmm.ucar.edu/models/wrf [Sep 2023].

Northern Ireland Environment Agency (2017) 'Guidance for Operators on producing an Air Dispersion Modelling Report for a PPC Farming Application'.

Oettl, D. (2016) 'Documentation of the prognostic mesoscale model GRAMM-SCI (Graz Mesoscale Model -Scientific)'.

OpenFOAM (2023) *Homepage*, [Online], Available: https://www.openfoam.com/ [Sep 2023].

OxAir (2021) 'OxAir Air Quality Sensor Pilot'.

Oxford Instruments (2023) *A new Imaging MAX-DOAS Instrument for Measuring Atmospheric Pollution*, [Online], Available: https://andor.oxinst.com/learning/view/article/a-new-imaging-max-doas-instrument-for-measuring-atmospheric-pollution [Sep 2023].

Paatero, P. (1997) 'Least squares formulation of robust non-negative factor analysis', *Chemometrics and Intelligent Laboratory Systems*, vol. 37, no. 1, pp. 23 - 35.

Peters, D.R., Papoola, O.A.M., Jones, R.L., Martin, N.A., Mills, J., Fonseca, E.R., Stidworthy, A., Forsyth, E., Carruthers, D., Dupuy-Todd, M., Douglas, F., Moore, K., Shah, R.U., Padilla, L.E. and Alvarez, R.A. (2021) 'Evaluating Uncertainty in Sensor Networks for Urban Air Pollution Insights', *Atmospheric Measurement Techniques Discussions*.

Pisso, I., Sollum, E., Grythe, Kristiansen, N.I., Cassiani, M., Eckhardt, S., Arnold, D., Morton, D., Thompson, R.L., Groot Zwaaftink, C.D., Evangeliou, N., Sodemann, H., Haimberger, L., Henne, S., Brunner, D., Burkhart, J.F., Fouilloux, A., J, B. and Philipp, A. (2019) 'The Lagrangian Particle Dispersion Model FLEXPART Version 10.4', *Geoscience Model Development*, vol. 12, pp. 4955 - 4997.

Price, C.S., Stocker, J., Johnson, K., Patel, R., Strickland, S., Doktarova, J. and Rubinis, J. (2021) 'A Review of Approaches to Dispersion Modelling of Odour Emissions and Intercomparison of Models and Odour Nuisance Assessment Criteria'.

Radiello (2023) *Radiello Samplers*, [Online], Available: https://radiello.com/ [Sep 2023].

Ramboll (2020) *User's Guide Compehensive Air Quality Model with Extensions Version 7.20*, [Online], Available: www.camx.com [Sep 2023].

Ricardo (2022) *AURN QA/QC Annual Technical Report 2021*.

Rohi, G., Ejofodomi, O. and Ofualagba, G. (2020) 'Autonomous monitoring, analysis, and countering of air pollution using environmental drones', *Heliyon*, vol. 6 (1), Available: https://www.sciencedirect.com/science/article/pii/S2405844020300979.

Rojas, A.J., Gonzalez, L.F., Motta, N. and Villa, T.F. (2015) 'Design and flight testing of an integrated solar powered UAV and WSN for remote gas sensing', 2015 IEEE Aerospace Conference, Big Sky, MT, USA, 1-10.

Russell, M., Hakami, A., Makar, P.A., Akingunola, A., Zhang, J., Moran, M.D. and Zheng, Q. (2019) 'An evaluation of the efficacy of very high resolution air-quality modelling over the Athabasca oil sands region, Alberta, Canada', *Atmospheric Chemistry and Physics*, pp. 4393-4417.

Sandu, A. and Chai, T. (2011) 'Chemical Data Assimilation - An Overview', *Atmosphere*, vol. 2, pp. 426-463.

Scire, J.S., Robe, F.R., Fernau, M.E. and Yamartino, R.J. (2000) *A user's guide for the CALMET Meteorological Model*, Earth Tech.

Scire, J.S., Strimaitis, D.G. and Yamartino, R.J. (1990) *Model formulation and user's guide for the CALPUFF dispersion model*, Concord, MA: Sigma Research Corp.

SEEDS (2023) *SEEDS data portal*, [Online], Available: https://www.seedsproject.eu/data [Sep 2023].

Siemens (2023) *Products*, [Online], Available: https://www.plm.automation.siemens.com/global/en/products/simcenter/STAR-CCM.html [Sep 2023].

Simpson, D., Benedictow, A., Berge, H., Bergström, R., Emberson, L.D., Fagerli, H., Flechard, C.R., Hayman, G.D., Gauss, M., Jonson, J.E., Jenkin, M.E., Nyíri, A., Richter, C., Semeena, V.S., Tsyro, S., Tuovineen, J.P., Valdebenito, Á. and Wind, P. (2012) 'The EMEP MSC-W chemical transport model-technical description', *Atmospheric Chemical Physics*, vol. 12, pp. 7825 - 7865.

Siour, G., Colette, A., Menut, L., Bessagnet, B., Coll, I. and Meleux, F. (2013) 'Bridging the scales in a eulerian air quality model to assess megacity export of pollution', *Environmental modelling & software*, vol. 46, pp. 271-282.

Stidworthy, A., Carruthers, D., Stocker, J., Balis, D., Katragkou, E. and Kukkonen, J. (2013) 'Myair toolkit for model evaluation', 5th International Conference on Harmonisation, Madrid, Spain, Madrid.

Stocker, J., Ellis, A., Smith, S., Carruthers, D., Venkatram, A., Dale, W. and Attree, M. (2016) 'A Review of the Limitations and Uncertainties of Modelling Pollutant Dispersion from Non-point Sources', in *Report fo rthe UK Atmospheric Dispersion Modelling Liaison Committee*.

Stocker, J., Ellis, A., Smith, S., Carruthers, D., Venkatram, A., Dale, W. and Attree, M. (2017) 'A Review of Dispersion Modelling of Agricultural Emissions with Non-point Sources', *International Journal of Environment and Pollution*, vol. 62, no. 2 - 4, pp. 247 - 263.

Sykes, R.I., Parker, S.F., Henn, D.S. and Lewellen, W.S. (1993) 'Numerical simulation of ANATEX tracer data using a turbulence closure model for long-range dispersion', *Journal of Applied Meteorology and Climatology*, vol. 32(5), pp. 929-947.

Takahama, S. (2015) 'pmf-tools: DOI Release (v1.0)'.

Targa, J., Loader, A. and Defra (2008) *Working group on Harmonisation of Diffusion Tubes*, [Online], Available: https://laqm.defra.gov.uk/documents/0802141004_NO2_WG_PracticalGuidance_Issue1a.pdf [Sep 2023].

The European Parliament and the Council of the European Union (2008) 'Directive 2008/50/EC of the European Parliament and of the Council of 21 May 2008 on ambient air quality and cleaner air for Europe', *Official Journal of the European Union*.

The Newsroom (2021) 'Log Burners in Bristol: Pollution Monitoring begins Amid Calls for a Ban', *Bristol World*.

The Royal Society (2018) 'The Impact of Ammonia Emissions from Agriculture on Biodiversity'.

UK Research and Innovation (2019) *Integrated Research Observation System for Clean Air (OSCA)*, [Online], Available: https://gtr.ukri.org/projects?ref=NE%2FT001798%2F1 [Sep 2023].

UK Research and Innovation (2022) *Area of Investment and Support: Clean Air*, [Online], Available: https://www.ukri.org/what-we-offer/browse-our-areas-of-investment-and-support/clean-air/ [Sep 2023].

UKCEH (2023) *Air Pollution Information System*, [Online], Available: https://www.apis.ac.uk/ [Sep 2023].

Ulbrich, I.M., Canagaratna, M.R., Zhang, Q., Worsnop, R. and Jimenez, J.L. (2009) 'Interpretation of organic components from Positive Matrix Factorization of aerosol mass spectrometric data', *Atmospheric Chemical Physics*, vol. 9, pp. 2891 - 2918.

United States Environmental Protection Agency (2022) 'The Enhanced Air Sensor Guidebook'.

United States Environmental Protection Agency (2023) *Positive Matrix Factorisation Model for Environmental Data Analyses*, [Online], Available: https://www.epa.gov/air-research/positive-matrix-factorization-model-environmental-data-analyses [Sep 2023].

University College London (2023) *Person Environment Activity Research Laboratory (PEARL)*, [Online], Available: https://www.ucl.ac.uk/pearl [Sep 2023].

University of Manchester: Centre for Atmospheric Science (2023) *Manchester Air Quality Super Site at the Firs Environmental Research Station, Fallowfield Campus*, [Online], Available: http://www.cas.manchester.ac.uk/restools/firs/ [Sep 2023].

Urban Flows Observatory (2020) *Air Pollution and the Air Quality Sensor Farm*, [Online], Available: https://urbanflows.ac.uk/air-quality-sensor-farm/ [Sep 2023].

van Jaarsveld, J.A. (2004) 'The Operational Priority Substances Model'.

van Zanten, M.C., Sauter, F.J., Wichink Kruit, R.J., van Jaarsveld, J.A. and van Pul, W.A.J. (2010) 'Description of the DEPAC Module', *Dry Deposition Modelling with DEPAC GCN2010*, pp. 1 - 76.

Vijayaraghavan, K., Snell, H.E. and Seigneur, C. (2008) 'Practical Aspects of Using Satellite Data in Air Quality Modeling', *Environmental Science & Technology*, vol. 42 (22), pp. 8187-8192, Available: https://pubs.acs.org/doi/10.1021/es7031339.

Vivid Economics (2022) 'Natural Capital Account - Bristol'.

Walters, D., Baran, A.J., Boutle, I., Brooks, M., Earnshaw, P., Edwards, J., Furtado, K., Hill, P., Lock, A., Manners, J. and Morcrette, C. (2019) 'The Met Office Unified Model Global Atmosphere 7.0/7.1 and JULES global land 7.0 configurations', *Geoscientific Model Development*, vol. 12, no. 5, pp. 1909 - 1963.

Wesely, M.L., Doskey, P.V. and Shannon, J.D. (2002) 'Deposition parameterisations for the industrial source complex (ISC3) model (No. ANL/ER/TR-01/003; W-31-109-Eng-38)'.

Whitehill, A.R., Melissa, L., Kaushik, and Solomon, (2020) 'Uncertainty in collocated mobile measurements of air quality', *Atmospheric Environment*, vol. 7, Available: https://www.sciencedirect.com/science/article/pii/S2590162120300198.

Williamson, T., Nunn, J. and Pearce, H. (2021) 'Air Pollution and Inequalities in London: 2019 Update, prepared for Greater London Authority', Available: https://www.london.gov.uk/sites/default/files/air_pollution_and_inequalities_in_london_2019_update_0.pdf.

World Meteorological Organisation (2023) *OSCAR Satellite: Metop-C*, [Online], Available: https://space.oscar.wmo.int/satellites/view/metop_c [Sep 2023].

Yusuf, S.N.A., Asako, Y., Sidik, N.A.C., Mohamed, S.B. and Japar, W.M.A.A. (2020) 'A short review on rans turbulence models', *CFD Letters*, pp. 12(11), 83-96.

Zefon (2021) *Passive vs. Active Air Sampling*, [Online], Available: https://www.zefon.com/passive-vs-active-air-sampling#:~:text=Passive%20Air%20Sampling,-Passive%20air%20sampling&text=This%20method%20may%20be%20deemed,gaseous%20and%20vapor%20molecules%20enter. [Sep 2023].

Zheng, Y., Miao, Y., Liu, S., Chen, B., Zheng, H. and Wang, S. (2015) 'Simulating flow and dispersion by using WRF-CFD coupled model in a built-up area of Shenyang, China', *Advances in Meteorology*.

List of abbreviations

ACSM	Aerosol Chemical Speciation Monitor
ACTM	Atmospheric chemistry transport model
ACTRIS	Aerosol, Clouds and Trace Gases Research Infrastructure
ADMLC	Atmospheric Dispersion Modelling Liaison Committee
ADMS	Atmospheric Dispersion Modelling System
AERMOD	American Meteorological Society and United States Environmental Protection Agency Regulatory Model
AI	Artificial intelligence
ALPHA	Adapted Low-cost Passive High-Absorption
ANN	Artificial neural network
APAS	Air Pollution Assessment Service
AQC	Air Quality Consultants Ltd
AQEG	Air Quality Expert Group
ASCENT	Atmospheric Science and Chemistry Measurement Network
AURN	Automatic Urban and Rural Network
AUSTAL	Ausbreitungsrechnungen nach TA Luft (dispersion model)
BOKU	Universität für Bodenkultur (University of Natural Resources and Life Sciences)
CALMET	CALPUFF meteorological preprocessor
CALPOST	CALPUFF post-processor
CALPUFF	California Puff (dispersion model)
CAMS	Copernicus Atmosphere Monitoring Service
CAVE	Controlled Active Ventilation Environment
CBED	Concentration Based Estimated Deposition (model)
CCUS	Carbon capture, utilisation and storage
CERC	Cambridge Environmental Research Consultants

CFD	Computational fluid dynamics
CIBSE	Chartered Institution of Building Services Engineers
CMAQ	Community Modelling Air Quality
CMB	Chemical mass balance
CO	Carbon monoxide
CTM	Chemical transport model
DEPAC	Deposition of acidifying compounds
Defra	Department for Environment, Food and Rural Affairs
DELTA	DEnuder for Long-Term Atmospheric sampling
DIAL	Differential Absorption Lidar
DL	Deep learning
DNS	Direct numerical simulation
DOAS	Differential Optical Absorption Spectroscopy
Dr-TAPM	Drone for Real-time Air Pollution Monitoring
EMEP	European Monitoring and Evaluation Programme
ESA	European Space Agency
EU	European Union
FDMS	Filter Dynamics Measurement System
FLEXPART	FLEXible PARTicle (dispersion model)
FTIR	Fourier transform infrared
GEMS	Geostationary Environment Monitoring Spectrometer
GRAL	Graz Lagrangian Model
H	Hydrogen
HCl	Hydrogen chloride
HF	Hydrogen fluoride
HYSPLIT	Hybrid Single-Particle Lagrangian Integrated Trajectory model

IR	Infrared
JNCC	Joint Nature Conservation Committee
LCS	Low-cost sensors
LES	Large eddy simulation
LPDM	Lagrangian particle dispersion model
LSTM	Long Short-Term Memory (networks)
MCDA	Multiple-criteria decision analysis
MCM	Master Chemical Mechanism
MIE	Model inter-comparison exercise
ML	Machine learning
MPI	Message passing interface
MTG	Meteosat Third Generation
NAMN	National Ammonia Monitoring Network
NCAS	National Centre for Atmospheric Science
NECR	National Emissions Ceiling Regulations
NERC	National Environment Research Council
NH_3	Ammonia
NO	Nitric oxide
NO_2	Nitrogen dioxide
NOx	Nitrogen oxides
NOAA	National Oceanic and Atmospheric Administration
NWP	Numerical weather prediction
O_3	Ozone
OML	Operationelle Meteorologiske Luftkvalitetsmodeller
OPS	Operational model for Priority Substances
OSCA	Observation System for Clean Air

OSPM	Operational Street Pollution Model
PM	Particulate matter
$PM_{2.5}$	Particulate matter with an aerodynamic diameter of ≤2.5µm
PM_{10}	Particulate matter with an aerodynamic diameter of ≤10µm
PMF	Positive Matrix Factorisation
QA	Quality assurance
QC	Quality control
RAL	Rutherford Appleton Laboratory
RANS	Reynolds-averaged Navier-Stokes
RDE	Research, Development and Evidence (Defra Framework)
RMSE	Root mean square error
RNN	Recurrent neural network
SAC	Special Area of Conservation
SCICHEM	Second-order Closure Integrated Puff (SCIPUFF) with Chemistry
SEEDS	Sentinel EO-based Emissions and Deposition Service
SEPA	Scottish Environment Protection Agency
SO_2	Sulphur dioxide
SOF	Solar Occultation Flux
SPA	Special Protection Area
SSI	Site of Scientific Interest
SSSI	Site of Special Scientific Interest
TDLAS	Tunable diode laser absorption spectroscopy
TEMPO	Tropospheric Emissions: Monitoring of Pollution
TEOM	Tapered element oscillating microbalance
TOMP	Toxic Organic Micro-Pollutant
TUM	Technische Universität München (Technical University of Munich)

UAV	Unmanned aerial vehicle
UEQ	Urban environmental quality
UFP	Ultrafine particle
$\mu g/m^3$	Microgrammes per cubic metre
UK-AQST	UK Air Quality Supersite Triplets
UKCEH	UK Centre for Ecology and Hydrology
UKEAP	UK Eutrophying and Acidifying Pollutants
US EPA	United States Environmental Protection Agency
UV	Ultraviolet
UV/vis	Ultraviolet/visible light
VOC	Volatile organic compound
WHO	World Health Organization
WRF	Weather research and forecasting

Would you like to find out more about us or your environment?

Then call us on

03708 506 506 (Monday to Friday, 8am to 6pm)

Email: enquiries@environment-agency.gov.uk

Or visit our website

www.gov.uk/environment-agency

incident hotline

0800 807060 **(24 hours)**

floodline

0345 988 1188 **(24 hours)**

Find out about call charges (https://www.gov.uk/call-charges)

Environment first

Are you viewing this onscreen? Please consider the environment and only print if absolutely necessary. If you are reading a paper copy, please don’t forget to reuse and recycle.