Ricardo
Energy & Environment

Ammonia futures: understanding implications for habitats and requirements for uptake of mitigation measures

Modelling workshop report

Report for Defra
ecm_53127

ED 11554 | Issue Number 1 | 03/07/2019

Customer:

Defra

Customer reference:

ecm_53127

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Date:

03/07/2019

Ricardo Energy & Environment reference:

Ref: ED11554- Issue Number 1

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Glossary of terms and abbreviations

Term / abbreviation	Explanation
ADMS	Atmospheric Dispersion Modelling System, a Gaussian dispersion model published by CERC; see Section 2.1
AERMOD	A Gaussian dispersion model developed by the United States Environmental Protection Agency (US EPA)
APIS	Air Pollution Information System (www.apis.ac.uk)
AQUM	Air Quality in the Unified Model; see Section 2.2
ASSI	Area of Special Scientific Interest, a UK protected area located within Northern Ireland or the Isle of Man.
AURN	Automatic Urban and Rural Network, the UK's largest automatic air quality monitoring network
CBED	Concentration Based Estimated Deposition; see Section 2.2
CEH	Centre for Ecology & Hydrology
CERC	Cambridge Environmental Research Consultants
CL	Critical Level (for airborne pollutants such as NH_3) or Critical Load (for deposition pollutants such as nitrogen deposition); pollution thresholds set for the protection of sensitive ecosystems
CLRTAP	Convention on Long-Range Transboundary Air Pollution
CMAQ	Community Multi-scale Air Quality (CMAQ) model; see Section 2.2
CTM	Chemical transport model; see Section 2.1
Defra	Department for Environment, Food and Rural Affairs
EMEP4UK	An application of the European Monitoring and Evaluation Programme (EMEP) model, adapted to the UK; see Section 2.2
Eulerian	A type of CTM; see Section 2.1
EU	European Union
FRAME	Fine Resolution Atmospheric Multi-pollutant Exchange, a Lagrangian CTM; see Section 2.2
Gaussian dispersion model	A type of atmospheric dispersion model; see Section 2.1
GCM	General circulation model; see Section 2.1
GHG	Greenhouse gas
H_2SO_4	Sulphuric acid, an acid which can react with ammonia in the atmosphere
HCl	Hydrochloric acid, an acid which can react with ammonia in the atmosphere
HNO_3	Nitric acid, an acid which can react with ammonia in the atmosphere
Lagrangian	A type of CTM; see Section 2.1
MetUM	Met Office Unified Model, a numerical model of the atmosphere used for weather and climate applications
NAEI	National Air Emissions Inventory, for the UK

Term / abbreviation	Explanation
NAME	Numerical Atmospheric dispersion Modelling Environment; see Section 2.2
NARSES	National Ammonia Reduction Strategy Evaluation System, the spreadsheet model preceding the current UK Agriculture GHG and Ammonia Emissions Inventory model
NECD	National Emissions Ceiling Directive
NH_3	Ammonia
NO_2	Nitrogen dioxide
NOx	Oxides of nitrogen, including nitrogen dioxide (NO_2) and nitrogen oxide (NO)
O_3	Ozone
PM_{10}	Particulate matter air pollution with a particle diameter ≤ 10 µm
$PM_{2.5}$	Fine particulate matter air pollution with a particle diameter ≤ 2.5 µm
Ramsar site	A wetland site designated to be of international importance under the Ramsar Convention.
SAC	Special Area of Conservation, a strictly protected site designated under the EC Habitats Directive.
SO_2	Sulphur dioxide, a gaseous compound which can react to form sulphuric acid in the atmosphere
SPA	Special Protection Area, a strictly protected site classified in accordance with Article 4 of the EC Birds Directive, which came into force in April 1979.
SSSI	Site of Special Scientific Interest, a UK protected area located within Great Britain.
UKIAM	UK Integrated Assessment Model; see Section 2.2
UNECE	United Nations Economic Commission for Europe
VOCs	Volatile organic compounds

1 Introduction

This report is the output of Work Package 2 of the project Ammonia futures: understanding implications for habitats and requirements for uptake of mitigation measures. It focusses on the outputs from a 1-day workshop relating to the modelling tools currently used for assessing the impacts of reactive nitrogen on terrestrial ecosystems.

Work Package 1 Report, *Ammonia futures: understanding implications for habitats and requirements for uptake of mitigation measures* gathered and collated information from stakeholders/farmers on co-benefits, trade-offs, local factors, and barriers to implementation and incentives to overcome barriers. This was done through a series of 13 regional (England) stakeholder workshops and is reported separately.

1.1 Policy context

The 25 Year Environment Plan sets out the ambition for improvements to the environment. Clear air and thriving plants and wildlife are specific goals within the plan that are directly affected by ammonia emissions. This workshop was designed to help assess the tools (models) available for policy use in assessing the impacts of reactive nitrogen on terrestrial ecosystems and human health. The usefulness of tools and potential limitations are determined by a range of factors including uncertainty, geographic and temporal granularity and flexibility as these all affect how tools measure progress against indicators and the effectiveness of policies.

The NECD requires the UK to report the impacts of air pollution upon ecosystems on an annual basis from June 2019. In 2015, 63% of UK's sensitive habitat exceeded nitrogen deposition critical loads (Hall, Smith and Dore 2017). This is predominantly from agricultural ammonia (NH_3) emissions, but NOx and long-range transport are also key.

Improvements in the evidence base for air quality will reduce uncertainty and inform policy evaluation and decision making.

1.2 Objectives

The objectives of Work Package 2 are listed below:

- Organise an academic expertise workshop to consider the appropriate data and state-of-the-art modelling tools for assessing the impacts of reactive nitrogen on terrestrial ecosystems, considering recent evaluations of their differences (Dore, et al. 2015).
- Provide a critical assessment of tools available for assessing likely impact of ammonia mitigation on protected UK sites and the spatial and temporal extent to which useful predictions can be made. This will include:
    - Estimates of uncertainty and the implications of this uncertainty for vegetation-specific nitrogen deposition in currently available models and those under development.
    - Limitations of calibration between models.
- Where possible guidance on suggested parametrizations and processes to be used for future model assessments of impacts of reactive nitrogen on terrestrial ecosystems.
    - Policy implications for the uncertainties and limitations identified.
- The workshop attendees should comprise model experts as well as experts from other environmental and numerate disciplines to provide peer review of the models, available data and to suggest appropriate levels of interpretation.

1.3 Introduction to ammonia as a pollutant

Current modelling capabilities in the UK can be described as multi-pollutant and multi-impact, as the main dispersion models used tend to model a wide range of pollutants, with impacts through multiple pathways including concentrations in air and deposition on land.

The modelling of NH_3 emissions and impacts is arguably more complex than modelling most other commonly-studied air pollutants due to a number of factors:

- Emissions are spatially and temporally complex, emitting from a variety of non-continuous agricultural processes which take place across a large number of small, discrete sources.
- NH_3 in the atmosphere is subject to complex chemical reactions which take place over a wide range of scales and timescales.
- NH_3 is removed from the atmosphere through complex depositional processes which take place over short timescales ranging from minutes to hours. Modelling of these depositional processes represents an important component of impact calculations.

As a result, a large number of tools are available for modelling NH_3 emissions and their dispersion in the atmosphere which approach the problem using different techniques. Different models focus on different time or spatial scales, and model treatment of emissions, chemistry and deposition can vary widely between models. Many models also provide advanced features representing particular aspects of NH_3 dispersion.

1.3.1 Emissions

Ammonia emissions derive from the breakdown and volatilization of urea and other sources of ammonium. The primary source of UK ammonia emissions is agriculture, accounting for 87% of UK emissions of ammonia in 2017 (Defra, 2019). Significant emissions arise from the application of manure, slurries and fertiliser, and from manure in animal housings. Emissions occur from a large number of small sources, including individual vents in housing units, and for this reason emissions can be modelled with a great degree of spatial detail if data is available with this resolution.

Unlike many other anthropogenic pollutant emissions, agricultural ammonia emissions are highly seasonal, with increased emissions occurring when manures and slurries are applied and when livestock are housed. On shorter timescales, changes in ambient temperature and wind speed lead to daily and seasonal variations in urea volatilization and ammonia emissions. However, national emission inventories tend to provide emissions as annual mean values provided over a grid with a resolution on the order of 1 to 10 km. Additional details on the UK emissions inventory are provided in Section 2.1.2.

Ammonia emissions within the UK peaked in the late 1980s and early 1990s. While emissions have had a mostly downward trend since then, this downward trend has recently reversed with emissions increasing by 10% between 2013 and 2017 (Defra 2019).

1.3.2 Chemistry

Ammonia in the atmosphere reacts quickly with acid gases to form aerosol-bound ammonium salts which add to background concentrations of fine particulate matter ($PM_{2.5}$). Two main reaction pathways occur:

- NH_3 reacts quickly with sulphuric acid (H_2SO_4) in the gas or aerosol phase to produce ammonium sulphate, $(NH_4)_2SO_4$. H_2SO_4 is formed through the oxidation of atmospheric sulphur dioxide (SO_2) by the hydroxyl radical or ozone. This process is generally considered to be irreversible.

- Reaction of NH_3 with nitric acid (HNO_3) or hydrochloric acid (HCl) will lead to an equilibrium between these gases and their aerosol phase ammonium salts. The equilibrium product is a function of the temperature and humidity.

As a result, the lifetime of gaseous ammonia in the atmosphere is typically a few hours. Because acid gases (sulphuric acid, nitric acid and hydrochloric acid) participate in the above reactions to remove ammonia from the atmosphere, concentrations of ammonia in the atmosphere will depend on the availability of acid gases as well as the magnitude of ammonia emissions. Aerosol-bound ammonium has a longer lifetime in the atmosphere and is primarily removed by wet deposition rather than dry deposition.

1.3.3 Deposition

Deposition of NH_3 occurs through dry deposition and deposition in precipitation (wet deposition). Dry deposition is the most important removal process; the rate of deposition is a strong function of the concentration of NH_3 at the surface and the physical, chemical and biological characteristics of the surface. Most models use one of two approaches to modelling dry deposition:

1. Modelling using a deposition velocity, which varies by pollutant and surface type. The deposition velocity is typically derived using a multiple-resistance approach allowing the user more control over deposition parameters and assumed conditions.
2. An empirical relationship between concentrations in air and deposition derived from measurements can be used.

Wet deposition occurs through uptake of NH_3 in cloud droplets (referred to as in-cloud scavenging) and uptake in precipitation (below-cloud scavenging). Wet deposition rate is a function of precipitation rate.

2 Workshop report

2.1 Modelling tools

2.1.1 Introduction to modelling approaches

The workshop provided an opportunity to gather together some of the key modelling groups and models that are capable of modelling emissions of NH_3 from source emission through to ecosystem impacts.

The models available include local scale models such as the suite of ADMS models (scales of up to 10s of km), empirically-based models such as CBED, and full chemical transport models (CTM) such as EMEP4UK, CMAQ, NAME and AQUM. These models can be categorised by a number of basic features, including:

1. Type (see below);
2. Spatial scale – grid size, requirements for nesting, vertical resolution;
3. Emission schemes;
4. Meteorology;
5. Chemistry scheme – level of chemical complexity with respect to NH_3.

A CTM is a model which simulates atmospheric chemistry on a regional or global scale. In contrast to GCMs (general circulation models), which focus on simulating overall atmospheric dynamics, CTMs focus on flows and budgets of chemical species. In recent years, the trend is for GCMs to incorporate CTMs in order to allow feedback between the two systems. CTMs are subdivided into Eulerian models and Lagrangian models:

- Lagrangian: Dispersion model mathematically calculates the trajectories of a large number of plume parcels. These models frequently use simpler approaches to meteorology, often using annual average meteorological data rather than dynamic meteorology. These models are faster to run, and as a result were favoured in the past in order to allow larger model domains to be modelled at higher resolutions.
- Eulerian: Similar to a Lagrangian model, pollutants are tracked from their source. However, a Eulerian model uses a three-dimension grid rather than following individual parcels. These models tend to include dynamic meteorology, allowing higher temporal and spatial resolution. However, Eulerian models are considerably more computationally expensive, and as a result model resolution and the complexity of chemical schemes can be limited by available computing resource, which has historically limited their applicability in short-field studies.

In the past, atmospheric modelling was typically undertaken using ‘simpler’ Lagrangian models such as FRAME, which operate in an annual average mode using average meteorological conditions. As computing power has increased, the use of more complex Eulerian meteorological models to drive chemical transport models has become feasible and more widespread. Many CTMs used in the UK use outputs from lower-resolution global models to provide boundary conditions outside the UK, with the UK being modelled at a higher resolution.

In addition to these regional CTMs, short-range models are available which allow detailed modelling of impacts from individual sources. Gaussian plume models assume that pollutant concentrations follow a normal distribution around the plume centreline, the trajectory of which is calculated using hourly meteorological data to calculate wind speed and turbulence profiles in the planetary boundary layer. Models typically calculate hourly dry and wet deposition fluxes based on simple schemes. Local dispersion effects such as plume rise, buildings, and variable surface roughness can also be taken into account. In the UK, commonly used Gaussian dispersion models include ADMS, published by CERC, and AERMOD, developed by the US EPA.

In addition to these detailed modelling approaches, a simpler class of models are available which use measurement-based estimates as the basis of an environmental assessment tool for past or present conditions. These models have very short run times, and as such are well-suited to the rapid assessment of large numbers of potential mitigation options. However, assessment of future scenarios typically requires detailed modelling using the tools described above, as estimates based on current emissions cannot account for changes in global temperatures. Measurements also have a limited spatial resolution, and as a result some tools combine measurement data with representative output from chemical transport models in order to provide gridded results.

2.1.2 UK Agriculture GHG and Ammonia Emissions Inventory

In the UK, NH_3 emissions from agriculture are compiled using the combined UK Agriculture GHG and Ammonia emission model (Misselbrook and Gilhespy 2019).

The UK Agriculture GHG and Ammonia Emissions Inventory models the flows of total nitrogen and total ammoniacal nitrogen (TAN) through the livestock production and manure management system. This approach has been adopted by the EMEP/EEA Guidebook as ‘best practice’. The Inventory model is built using a bottom up approach, using an activity data approach where:

Emission = Activity x Emission factor

Emission factors are derived, where possible, from measurements performed in the UK. It was noted that many measurements are dated, and updates may be useful where management practices have changed. Activity data for the UK is compiled from a wide range of sources depending on the sector, including livestock numbers, fertiliser use and other management practice data. Input resolution for activity data varies by activity. For example, livestock numbers are obtained at agricultural holding level, updated annually based on returns to the June Agricultural Survey (UK-wide) and the Cattle Tracing Scheme database (for England, Wales and Scotland) (Richmond, et al. 2019). By comparison, data related to management approaches are less resolved. Temporal resolution also varies by activity. For example, the model uses monthly rainfall to calculate emissions from grazed livestock (with the exception of sheep) and urea fertilizer application, but not for the application of slurry and manures, due to the large variability in activity data for management practices.

The UK Agriculture GHG and Ammonia Emission Inventory is a component of the larger UK National Atmospheric Emissions Inventory (NAEI) programme. The non-agricultural ammonia inventory follows a similar bottom up approach to estimate total UK ammonia emissions from nature, waste disposal and other miscellaneous sources (Tomlinson, et al. 2018). The methodology of the UK emissions inventories has primarily been driven by reporting requirements for the National Emissions Ceilings Directive (NECD) and the United Nations Economic Commission for Europe (UNECE) Convention on Long-Range Transboundary Air Pollution (CLRTAP). For inventory reporting purposes, emissions are provided as gridded emissions at 10 km resolution, disaggregated temporally (monthly) and by sector.

Emissions from the inventory models can subsequently be transferred to other models for dispersion and deposition modelling. For some modelling applications, emissions can be supplied at higher spatial resolutions to investigate more localized issues, such as predictions of ammonia concentrations and nitrogen deposition in the vicinity of sensitive habitats. Current limits to higher resolution emission models include: the spatial resolution of available source data (as discussed, some data such as livestock numbers are available at high spatial resolution, while other data is only available at low resolution); confidentiality requirements (while some data can be obtained at the level of individual agricultural holdings, these are typically aggregated into groups of at least 5 agricultural holdings in order to maintain anonymity); and resource constraints regarding the cost and time required to obtain more detailed datasets.

2.2 Comparison of model capabilities

2.2.1 Lagrangian chemical transport models

2.2.1.1 FRAME

The FRAME (Fine Resolution Atmospheric Multi-pollutant Exchange) model is a Lagrangian atmospheric transport model run by CEH on behalf of Defra to calculate annual averages of SO_x, NO_x and NH_x wet and dry deposition at a 5 km x 5 km resolution (although 1km resolution is also possible). The model uses static meteorology to calculate annual average concentrations and deposition fluxes. The vertical resolution of the model is extremely detailed, varying from 1m at the surface to 100m at the top of the domain.

Annual emissions of ammonia are estimated for each 5 km grid square using national data on farm animal numbers (cattle, poultry, pigs and sheep) as well as fertiliser application, crops and non-agricultural emissions (including traffic and contributions from human sources, wild animals etc). While some data is available at the level of individual farms, these are typically aggregated into groups of at least 5 farms in order to anonymise June Agricultural Survey data.

The FRAME chemistry scheme is similar to the scheme used in EMEP, and includes ammonium aerosol chemistry. Dry deposition is calculated individually in each grid square using a resistance model applied to five land use classes. Wet deposition is calculated using average precipitation rates (a constant drizzle approach), using a single scavenging coefficient based on EMEP.

2.2.1.2 UKIAM

The UK Integrated Assessment Model (UKIAM) has been developed by Imperial College London to rapidly investigate cost effective strategies for reducing UK emissions while maximising improvements in environmental protection in the UK. At the time of writing, the current version is 5b.

While not a chemical transport model, UKIAM uses source-receptor footprints from the FRAME model as part of its calculations. The other drivers are emissions, abatement costs for potential measures, and environmental criteria.

UKIAM brings together information on projected UK emissions of SO_2, NO_2, NO_X, NH_3, CO_2, N_2O, CH_4, PM_{10} and $PM_{2.5}$ to calculate the simultaneous effect of abatement measures on a combination of pollutants, and comparison of future scenarios.

2.2.1.3 NAME

NAME (Numerical Atmospheric dispersion Modelling Environment), first developed by the UK Met Office in 1986, is an off-line 1-way coupled Lagrangian-Eulerian dispersion and chemical transport model.

Like AQUM, NAME uses temporally-evolving meteorological data from the Met Office Unified Model (MetUM). The model provides forecasting, and model predictions are verified by comparison with all AURN stations, with observations feeding back to improve predictions such as for the influx of Saharan desert dust.

NAME includes a chemistry scheme including 34 transported species, 97 gas-phase and 19 photolysis reactions. Calculation of wet deposition includes in-cloud and below-cloud scavenging using a three-dimensional time evolving cloud and precipitation. Dry deposition rates are calculated using a multi resistance approach incorporating surface properties at 9 resolutions.

2.2.2 Eulerian chemical transport models

2.2.2.1 AQUM

AQUM (Air Quality in the Unified Model) is a limited area configuration of the Met Office Unified Model (MetUM), a Eulerian atmospheric chemistry forecast model which runs at 12km resolution over a domain covering the UK and Western Europe, producing a five-day air quality forecast.

The model uses the UKCA-RAQ chemical scheme, including 43 transported species, 116 gas-phase and 23 photolysis reactions, and includes removal by dry deposition and wet deposition. Aerosols are modelled using the CLASSIC scheme, which includes 8 aerosol types including ammonium sulphate and ammonium nitrate.

Dry deposition is modelled via a multiple resistance approach with surface resistance terms calculated for each tile. The resistances are calculated based on the roughness length, canopy height and surface heat flux. Wet deposition is parameterised as a first order loss rate, calculated as a function of the model's three-dimensional convective and large-scale precipitation.

2.2.2.2 CMAQ

The Community Multi-scale Air Quality (CMAQ) model is a Eulerian chemical transport model developed by the US EPA. Designed as a "one-atmosphere" model, CMAQ can model air quality issues simultaneously across spatial scales ranging from local to hemispheric. CMAQ allows a number of different chemistry and deposition schemes to be used, incorporating a wide range of reaction mechanisms and species. CMAQ is used by Ricardo Energy & Environment on behalf of Defra to calculate daily air quality forecasts for the UK. CMAQ is also used by other organisations, both within the UK and globally.

CMAQ includes several advanced features for modelling NH_3 and reactive nitrogen species, including a bidirectional flux option to simulate canopy resistance. Using this option, which requires use of the optional Environmental Policy Integrated Climate (EPIC) model to provide model parameters, the total flux between the plant canopy and overlying atmosphere is equal to the sum of:

- Two bidirectional pathways to the leaf stomata and soil; plus
- One uni-directional deposition pathway, to the leaf cuticle.

2.2.2.3 EMEP4UK

The European Monitoring and Evaluation Program Unified Model for the UK (EMEP4UK) is run by CEH, and is a Eulerian chemical transport model based on the EMEP MSC-W model, using a 5 km by 5 km British Isles grid nested within the EMEP 50 km x 50 km domain. The default vertical resolution is ~90 m at the surface, decreasing with height.

Pollutants simulated include PM_{10}, $PM_{2.5}$, elemental carbon, secondary organic aerosols, secondary inorganic aerosols, SO_2, NH_3, NOx, and O_3. The model uses the EmChem09 chemical reaction scheme to output more than 80 species including NH_3 and secondary aerosols. Dry deposition is modelled using a multiple resistance formulation, providing land-type specific deposition. Wet deposition includes both in-cloud and sub-cloud scavenging.

For the UK, emissions are taken from the National Atmospheric Emission Inventory (NAEI) at 1 km x 1 km resolution and aggregated to 5 km x 5 km resolution. For the rest of the European domain, the model uses the EMEP 50 km x 50 km resolution emission estimates provided by the EMEP Centre for Emission Inventories and Projections (CEIP).

2.2.3 Gaussian (short-range) models

2.2.3.1 ADMS

ADMS 5 (Atmospheric Dispersion Modelling System), developed by CERC (Cambridge Environmental Research Consultants), is an advanced Gaussian plume model designed for local-scale modelling of emissions from industrial sources, including emissions from agriculture.

The model operates on a short time scale as well as a short spatial scale (up to 50 km) compared with chemical transport models, and uses a steady-state assumption to calculate dispersion. The model includes features to model time-varying emissions sources, and allows discrete emission sources to be treated separately either as point sources or as passive volume sources, allowing concentrations to be calculated at metre-scale. ADMS is therefore designed for modelling of single farms, or small groups of farms.

ADMS 5 can calculate dry and wet deposition, and users can put in a spatially-varying deposition velocity field as well as a temporally varying field. This feature was the result of discussion with regulatory bodies in the UK.

2.2.4 Empirical models

2.2.4.1 CBED

The Concentration Based Estimated Deposition (CBED) model, run by CEH, is an empirical model which produces 5 km by 5 km resolution maps of pollutant concentrations, dry deposition, and wet deposition of pollutants including ammonia. Ammonia concentrations are derived from a combination of annual measured concentrations from the UK Eutrophying and Acidifying Pollutants (UKEAP) network, and the FRAME chemical transport model, which generates local scale variability that cannot be derived from the network measurement data. Data are calculated on an annual basis but provided as rolling 3-year means.

Dry deposition flux is calculated using spatially distributed estimates of habitat-specific deposition velocities for 5 land cover categories: forest, moorland, grassland, arable and urban.

Wet deposition includes deposition from precipitation as well as direct deposition of cloud droplets to vegetation (known as ‘occult’ deposition) and is mapped for sulphate, ammonium, nitrate, calcium, magnesium, and acidity (hydrogen ion).

2.3 Summary of model capability

Table 1: Basic information for each model considered in this report

Model	Model type	Meteorology	Deposition	Chemistry	Resolution	Typical application	Scale
Agriculture GHG & ammonia Model	Coded emissions inventory model	Annual average	N/A	N/A	Activity data from farm scale to GB-scale; output with a 10 km x 10 km grid resolution.	Develops emissions data for inventory purposes. Can provide improved input data for other models with improved livestock data at geographic and temporal scale.	UK
FRAME	Lagrangian CTM	Annual average	Dry: Deposition velocities calculated for 5 land types Wet: Constant drizzle approach	Similar to the scheme used in EMEP, and includes ammonium aerosol chemistry.	5 km x 5 km grid High vertical resolution, particularly at the surface	Run by CEH on behalf of Defra to calculate annual averages of SOx, NOx and NHx wet and dry deposition at a 5 km x 5 km resolution. Also used in UKIAM and CBED.	UK
UKIAM	Integrated Assessment Model	Annual average	Based on FRAME	Based on FRAME	5 km x 5 km grid	Incorporates emissions data from National Atmospheric Emissions Inventory (NAEI) and concentrations and deposition from the FRAME model to assess impacts of measures to reduce environmental impact.	UK
NAME	Lagrangian CTM	Dynamic	Dry: Multiple resistance model Wet: rainout and washout calculated using a 3-dimensional time evolving cloud and precipitation	Air quality based chemistry scheme including 36 reactive species	10 km horizontal	Used by the Met Office to model atmospheric dispersion events (i.e. smoke from fires, chemical accidents, etc.). The model can be run for both forward (predictive) and inverse (source identification) simulations.	Global to Local

Model	Model type	Meteorology	Deposition	Chemistry	Resolution	Typical application	Scale
AQUM	Eulerian CTM	Dynamic	Dry: Multiple resistance model calculated by tile Wet: First-order loss rate calculated from dynamic model precipitation	UKCA-RAQ reaction scheme; CLASSIC scheme for aerosols	12 km horizontal 40 km vertical	Used by the Met Office for short term forecasts of weather and air quality.	UK and European
CMAQ	Eulerian CTM	Dynamic	Dry: Multiple resistance model, including optional bidirectional flux model Wet: In-cloud and below-cloud scavenging	Multiple models available	Global-to-local	Can focus on sector or pollutant-based emissions and deposition. Can be used as a predictive tool.	Global to Local
EMEP4UK	Eulerian CTM	Dynamic	Dry: Surface-dependent multiple resistance model Wet: In-cloud and below-cloud scavenging	Incorporates 3D chemistry output of more than 80 species including ozone, NO_2, particulate matter, secondary inorganic/organic aerosols.	Global-to-local	Detailed modelling to provide assessments of critical load exceedances, and assess impacts of different policy scenarios on a wide range of pollutants.	Global to local
ADMS	Local-scale, Gaussian plume model	Hourly	Dry: Default values for deposition velocity, or user-specified parameters to estimate deposition velocity Wet: Single scavenging coefficient	Local-scale model, no explicit treatment of NH_3 chemistry	Metre resolution horizontally; Inside planetary boundary layer	Local-scale dispersion model used to model the air quality impact of existing and proposed industrial installations.	Typically 10s of km
CBED	Empirical	Annual average	Dry: Uses interpolated concentration maps and vegetation-specific deposition velocities (via a modified big leaf model)	Empirical	FRAME data used to provide 5km x 5km gridded output	Using the UK national measurement site concentration data, a concentration map for the UK is derived for SO_2, NO_2, HNO_3, NH_3, SO_4, NO_3 and NH_4. Deposition maps are also	UK

Model	Model type	Meteorology	Deposition	Chemistry	Resolution	Typical application	Scale
			Wet: Uses interpolated concentration maps and rainfall data from the UK Met Office			derived for acid and nutrient nitrogen deposition.	

2.4 Summary of workshop discussion on modelling tools

The morning session of the workshop included presentations providing an overview of the modelling tools currently available in the UK. Discussions relating to these presentations are summarized below.

2.4.1 Temporal and spatial variation in NH_3 emissions and modelling

Agricultural ammonia emissions fluctuate throughout the season depending on agricultural activities; these activities can vary from year to year depending on a range of factors affecting farm practices (often weather related); ammonia emissions from manure, slurries and fertilizers can result in short-term peaks in the spring and summer, whereas emissions from animal housing predominantly contribute to ammonia released throughout the housed period. The location and intensity of emissions at a farm change with the seasons. A question was raised during the workshop relating to how this temporal and spatial variation can be accounted for in the modelling process, and how these variations might affect the prioritization of mitigation measures.

There was general consensus that the variability of NH_3 emissions could theoretically be better captured during the modelling process, in that most modelling systems have a way to input some time variability associated with a particular emission source, down to a minute-by-minute resolution in some cases. However, one of the main difficulties in capturing this level of detail in the modelling process is a lack of time-resolved emission information, as many emission factors used in the UK’s agricultural GHG and ammonia inventory are annual averages although there are relevant elements that can be provided with greater temporal resolution. Some emission factors are modified according to climate, such as those used for inorganic fertilisers (modified on a monthly basis) and for spreading organic manures (on a summer and non-summer basis). Most activity data are available on a monthly or annual basis.

Spatial variation of NH_3 emissions is also limited by the availability of detailed emission inventories. The emissions from a specific farm depend on factors such as the type of farm, number and type of animals, size and type of crop fields, management practices, etc. Some of this information is relatively easy to obtain, such as the number of animals on a farm; however, other information, for example concerning management practices, is much more difficult to obtain. Information gathering and modelling with farm-by-farm levels of detail can be difficult for a number of reasons, including confidentiality issues in terms of collecting and sharing data, costs associated with gathering and collating data, etc. One suggestion was the use of a public register for farmers to record some useful information about their farm management practices, which could possibly be combined with a tool to allow farms to investigate ways of reducing the emissions from their farm.

In terms of how temporal and spatial variation might affect the prioritisation of mitigation measures, there was a general consensus that a better spatial understanding of emissions would be very beneficial, particularly in terms of targeting mitigation measures around sensitive habitat sites. In terms of temporal variability, the CL (critical level) values for NH_3 concentration, as well as for deposition of nutrient nitrogen and acid (of which NH_3 is a component) are all set on an annual basis. It was generally considered that the use of annual CL values is currently appropriate, partly due to the lack of information regarding the temporal variation of NH_3 emissions. If the temporal variation of NH_3 emissions could be captured with greater certainty, then consideration could be given to the development of short-term (daily or hourly) as well as long-term (annual) CL values. There was general consensus that although airborne NOx currently has an annual CL as well as a daily CL for the protection of sensitive habitats, in practice the annual CL is statistically more stringent for relating to effects on habitat. Additionally, it is unlikely that the daily CL will be exceeded if there is compliance with the annual CL or that the circumstances for inhibitory growth of plants from NOx would be met (e.g. simultaneous exceedance of CL for ozone and sulphur dioxide) (World Health Organization 2000).

2.4.2 Selection of meteorological information

Emissions of NH_3 depend on factors such as ambient temperature and humidity, although CL are set to be applied across a variety of environmental conditions (World Health Organization 2000). There was some discussion regarding the selection of meteorological datasets for modelling purposes. The selection of meteorological data depends on the purpose of the modelling study, and different decisions are appropriate for different modelling purposes.

- The UK Agriculture GHG and Ammonia Emissions Inventory model uses 30 year meteorological data averaged between 1981 and 2010 in order to have a consistent baseline with which to report progress against NECD targets. This is appropriate when it is important to have a consistent baseline, for example, to assess the effectiveness of mitigation measures in terms of reducing a metric such as fertilizer application. By modelling all scenarios with the same meteorological dataset, any changes in the model results are due to differences in metrics such as fertilizer application only and not due to variations in weather. However, the volatilization of urea and resulting ammonia emissions depend on factors such as ambient temperature. It would also be useful to have a set of ammonia emission outputs that are reflective of current or predicted weather trends (as appropriate) to be used in further dispersion and deposition models although the required updates and sophistication in processing data are likely to be challenging,
- For CBED results predicting deposition (including ammonia) on the Air Pollution Information System (APIS, www.apis.ac.uk), a three-year meteorological average is used to predict the deposition. This value is for a particular grid square used for assessing a plan or project effect on a designated site. This accounts for year on year variation when applying annual standards such as critical load or level.
- In other cases, it may be more appropriate to run a duplicate model using meteorological data corresponding to the year of the activity data so nitrogen deposition can be modelled more accurately. However, with this approach, it would be difficult to determine if year-to-year fluctuations in ammonia concentration and nitrogen deposition are due to fluctuations in emission sources, meteorological patterns, or a combination of both.
- Given the sensitivity of atmospheric ammonia reactions to temperature and humidity, it may also be informative to model future scenarios using a meteorological dataset that is designed to reflect anticipated changes to climate.

2.4.3 Possible improvements to the modelling process

There was general consensus that it was useful to bring together experts in different modelling systems for a discussion specifically related to modelling of NH_3 emissions, resulting air concentration and deposition when considering effects on habitat. Further discussions or studies focusing on the technical aspects of the modelling process, focusing on key tasks along the modelling chain, could be useful to develop improvements to the modelling of NH_3 and estimating effects on ecosystems.

It was also pointed out that verification of model performance is currently limited by the relatively low number of NH_3 monitoring locations in the UK. There are fewer locations that monitor NH_3, compared to other pollutants such as NOx and PM_{10}. Furthermore, many of the locations that currently monitor NH_3 only provide annual average mean concentrations. Additional monitoring locations for NH_3, and in particular locations that provide hourly NH_3 measures, would assist in verifying and improving model performance.

2.5 Summary of workshop discussion on suitability of models and strategies

The afternoon session of the workshop included discussions that were guided by specific questions. Comments and observations in response to the questions are detailed below.

2.5.1 How might we best predict where to target emissions reductions to deliver the greatest impact on the environment?

This is a key question and an active area of research. Recent projects in this area have: investigated future trends in ammonia emissions across the UK and the potential benefits offered by targeted mitigation (Centre for Ecology & Hydrology, Rothamsted Research, Imperial College 2012), evaluated the effectiveness of current and past agri-environment schemes in delivering air quality improvements (Carnell, et al. 2018), and identified potential remedies for air pollution (nitrogen) impacts on designated sites (Dragosits, et al. 2015). While the NECD commits the UK to reducing total emissions of ammonia, among other pollutants, more information is needed to guide policy and mitigation measures in order to maximise the benefits for protected habitat sites.

When considering the impact side, there is a need to consider what is meant by a sensitive site. Currently, designated sites with European (or equivalent international) designation, namely Ramsar sites, Special Areas of Conservation (SACs) and Special Protection Areas (SPAs), have high levels of protection through the Conservation of Habitats and Species Regulations 2017 (‘the Habitats Regulations’). There are other sites of national importance and local importance which can be considered sensitive sites although they do not fall under the Habitats Regulations, including Sites of Special Scientific Interest (SSSIs), Areas of Scientific Interest (ASSIs), National Parks, etc. There is also some uncertainty regarding how environmental legislation may change after an exit from the EU.

There is also a need to consider what the priorities are for the protection of sensitive sites – i.e., are all sensitive sites given equal priority, do we prioritize reducing pollution impacts at sites with the greatest amount of existing air pollution, do we focus on protecting those sites that are not yet damaged, etc.? Despite the protection offered by the Habitats Regulations, many European-designated sites are currently in exceedance of the applicable critical levels and critical loads (Hall, Smith and Dore 2017). There was a general consensus that we have a duty to restore areas of designated sites which are already in a poor condition due to air pollution impacts, while also protecting those sites which are not damaged. Although undamaged sites may be considered to have ‘more headroom’ before they are damaged by air pollution and could therefore be seen as lower priority in terms of protection, these sites should not be allowed to degrade to the point where they are damaged; recovery of damaged sites is slow, difficult and expensive.

Whilst agreed as an objective, there is no single UK policy to restore damaged sites and to protect undamaged ones. Section 2.6 explores this further. Environment is a devolved matter and this policy objective is tackled in many ways. England has its Clean Air Strategy 2019. Wales has a cross-cutting Well-being of Future Generations Act. It was mentioned that Northern Ireland has a banding system in place for high risk areas, and that might be an approach that is useful elsewhere in the UK. Scotland is investigating approaches targeted at reducing the number of large poultry and dairy farms in areas where NH_3 concentrations are high.

Once priority areas are identified, atmospheric modelling could be used for source apportionment of NH_3 emissions and concentrations into different sectors. The APIS website includes source apportionment information on the Source Attribution tab of the Site Relevant Critical Loads pages, however, the source apportionment is based on emissions data from 2012 and may not reflect recent changes in emissions from different sectors. The understanding of source apportionment could be improved by using more recent emissions data and/or by improving the spatial resolution of the emissions inventory. The latter would require improved localised information about NH_3 sources and emission rates. Source apportionment information could be used to look at the cost of abatement options and prioritize those options considered to be most cost-effective. It was pointed out that it may be difficult to obtain or derive financial values for environmental damage, whereas more research has already been done in this area in relation to the cost of damage to human health. Although financial values for environmental damage may not be easy to obtain, there is existing information on exceedances of annual critical levels and critical loads, which can be related to location-specific habitats (Hall, Smith and Dore 2017), and this information can be used to prioritize mitigation options in terms of environmental benefit. For related discussion, See Section 2.2.3.4 Environmental Benefit in the report for Work Package 1.

It was suggested that a minimum environmental benchmark could be implemented for all farms to achieve. Depending on how the benchmark is defined, i.e. in terms of total NH_3 emissions or in terms of impacts on nearby sensitive habitats, farms that are located near or next to a sensitive receptor site would have to do more in terms of implementing mitigation measures. A future opportunity may be for a modelling tool to support an outcome-based approach, with farmers using a system to input information and receiving an output with the results. However, this may be challenging to implement and would be difficult to monitor, particularly if farmers and other ammonia emitters are unable or unwilling to input accurate information.

It was suggested that more research is required to determine the long-term effects of ammonia emissions and concentrations, including the health hazards, in order to identify the areas that need to be targeted and to promote uptake by the agricultural community.

When considering policy and mitigation options to deliver environmental benefits to protected habitat sites, it is important to consider the spatial analysis capability of the different modelling approaches. All of the models discussed in this report can provide spatial analysis at some scale. The resolution of the spatial analysis, and any subsequent assessment of impacts on specific designated sites or portions of designated sites, depends on several factors including:

- The resolution of the available input data. As discussed in Section **Error! Reference source not found.**, the spatial resolution of activity data incorporated in the UK Agriculture GHG and Ammonia Emissions Inventory, and in the greater NAEI, varies by activity. The outputs are typically gridded at a 10 km resolution for emissions reporting. However, this may be too coarse a resolution for input into dispersion and deposition models when assessing impacts on the scale of designated sites, as the majority of designated sites are smaller than one 10 km x 10 km grid square. In order to assess impacts and improvements at the scale of designated sites, higher resolution input data would be beneficial. Higher resolution input data is available for some datasets (such as numbers of livestock) but not for others (such as management practices).
- A trade-off between the model domain (or study area) and the model resolution. The computational cost of a model run increases as the study area increases and as the spatial resolution of the outputs increases. Due to computational and time constraints, model outputs covering all of the UK as a model domain will typically have output resolutions on the order of 5 to 10 km grids. Modelling studies focusing on a smaller model domain can be run at higher resolution, and some local-scale modelling studies can achieve resolutions of 1 m x 1 m, depending on how the model is set up.

- The resolution of datasets containing the spatial distribution of different types of habitat. The deposition of ammonia depends on the characteristics of the receiving environment, which will affect model parameters such as deposition velocity.

Apart from the UK Agriculture GHG and Ammonia Emissions Inventory model, which produces outputs on the basis of emissions rather than concentrations, all of the models discussed in this report provide outputs in terms of concentration and/or deposition, which can subsequently be related to the critical loads and critical levels of designated sites. Generally speaking, improvements can be made to the spatial analysis and impact assessment process by improving the resolution of input data, nesting local-scale models within larger-scale models, and improving the resolution of datasets used in the impact assessment step.

2.5.2 How best to attribute/apportion modelled change to specific policy measures and interventions?

Models can be useful tools to evaluate policy measures and interventions. However, the real world is complicated and there is a need to carefully consider both how scenarios are defined and how outcome indicators are assessed. There is a general risk that the outputs assessed by a given model or policy analysis tool could be too narrowly defined to capture unintended negative effects. Fuel choice for vehicles serves as a recent example of this. If petrol and diesel are assessed strictly in terms of reduction in greenhouse gas emissions, then diesel performs significantly better than petrol. However, if air quality is assessed alongside greenhouse gas emissions, then it becomes clearer that while diesel offers benefits in terms of reductions to some greenhouse gas emissions, it also has unintended negative impacts on air pollution.

One approach to try to minimize this risk would be to develop test case scenarios that comprise a suite of policy measures and interventions (rather than a single measure at a time) and assess the outputs across a wide range of indicators. This offers the advantage of potentially being able to capture interactions between measures and identify possible unintended effects; however, the scenarios and models themselves would be more complicated to develop and there is still a chance that an important interaction between measures would be left out or incorrectly modelled.

Two general methods of addressing the complexities of modelling the effects of policy measures and interventions were discussed:

- Beginning with simple models, possibly based in Microsoft Excel, and using these as a screening process to consider different scenarios, different combinations of measures, etc. Scenarios and combinations of measures which provide promising results in this screening phase can then be taken forward and developed into fuller scenarios using more sophisticated models.
- Developing an emulator based on the results of a more complicated model. The complicated model would be designed to try to accurately account for a complex range of variables and interactions between measures, and to output a range of indicators. Such a model would likely be computationally expensive to run; however, a few full scenarios could be run using this complicated model, and the results of these model runs could be used to set the bounds of a simpler emulator model. By interpolating between the results of the complicated model, the emulator can allow a greater number of scenarios to be explored in a shorter timeframe and can serve as a decision-making tool.

Regardless of the approach taken to model and assess the impacts of policy measures, it is important to improve our understanding of what specific models do well and what they struggle to do. This would put the model results into context, highlight risks associated with their use, and possibly improve stakeholder confidence in the process. It was pointed out, for example, that many farmers would potentially be interested in reducing their NH_3 emissions in order to improve the environment around them, and not just for personal financial reasons such as savings associated with using less fertiliser. In that case, it would be disheartening if there was a large discrepancy in terms of the magnitude of environmental improvements predicted by a model and the improvements that were achieved in the real world. Model accuracy could encourage greater uptake of mitigation measures, if people have confidence that the changes they are making will lead to real world improvements for the environment.

It was pointed out that source apportionment and attribution for a reactive species like ammonia can be difficult, particularly when it comes to attribution for secondary species. One approach would be to undertake apportionment/attribution studies of the precursors, which then requires a careful understanding of the chemistry involved and the use of a model that can accurately account for that chemistry. It was also pointed out that even for cases of simpler source apportionment involving primary pollutants, the uncertainty in activity data leads to uncertainty in model predictions and is a limiting factor in being able to attribute specific effects (i.e. reduction of ambient NH_3 concentrations) to specific mitigation measures.

There was a suggestion that semi-volatile amines should be given more consideration going forward. These species are currently not included in the national emissions inventory and are generally overlooked in modelling studies and policy evaluation. Nonetheless, they play an important role in the nucleation process for particulate matter formation.

2.5.3 What are the potential opportunities for doing things differently if the UK leaves the EU in terms of measurements and modelling?

There was limited discussion relating to this specific question.

Earlier in the workshop, a presentation from Defra referred to Article 9 of the National Emission Ceiling Directive (Revised NECD, 2016), which indicates that member states "…shall ensure the monitoring of negative impacts of air pollution upon ecosystems based on a network of monitoring sites that is representative of their freshwater, natural and semi-natural habitats and forest ecosystem types, taking a cost-effective and risk-based approach." Defra has indicated that they are committed to protecting the UK's sensitive ecosystems after the UK exits the EU, although the specific details of the approaches taken within the UK may differ after the EU exit. There may be opportunity to customize the protective approaches to be more specific to the UK.

2.5.4 What developments exist e.g. satellite measurements to aid model development, validation and interpretation?

Earlier in the day, there was some discussion of the need for improved understanding of the spatial distribution of different types of sensitive species and habitats within the larger boundary of a designated site. Models can be used to predict impacts on air quality (i.e., concentration of NH_3 in the air, deposition rate of nutrient nitrogen to the surface, etc.) at specified points, and there is uncertainty in the modelling process itself, as discussed elsewhere in this report. However, there is also uncertainty involved in interpreting those model results, in terms of understanding what species and/or habitats exist at the specified points. Some species and habitats are much more sensitive to air pollution impacts than others, and there is a need to understand the spatial distribution of species and habitats in order to interpret the model results. Mapping out every designated site using in-person site surveys would be time-intensive and costly.

One approach to address this data gap would be an increased use of satellite imagery for mapping designated sites. This is an approach currently being explored by Natural England through initiatives such as the ‘Living Maps’ project (Kilcoyne 2017). The overall goal is to develop a cost-effective method for creating broad-scale habitat maps derived from earth observation data, combined with ancillary datasets and mathematical models to predict the probability of a given habitat class occurring at a given location. Living maps, or similar, could then be used to provide greater certainty in assessing the effects of air pollution on sensitive species and habitats.

Other initiatives could focus on increasing public engagement alongside mapping out ecosystems and air quality impacts. An example of this would be the OPAL Air Survey (Imperial College London 2016), which encouraged members of the public to learn about air pollution while identifying the locations in their areas with lichens present on trees.

The concept of impact modelling on ecosystems was discussed. Dispersion modelling provides information from the perspective of air pollutants, their emission sources, and their fate in the atmosphere or as deposited to a surface. Impact modelling would provide information from the perspective of an ecosystem, accounting for information such as the soil type, the soil chemistry, the recovery rate of the ecosystem following a drop-off in air pollution levels, etc. Such a modelling approach would need to be dynamic and account for nitrogen turnover within the ecosystem.

2.6 Perspectives from devolved administrations

Policy context provided by Defra has been summarized in Section 1.1. At the workshop, representatives from each of the devolved administrations provided their own perspectives on NH_3 issues, summarized below.

2.6.1 Wales (Ji Ping, NRW)

- The Welsh government are aiming for a farm support program for NH_3 in agriculture, targeting sectors considered high ammonia emitters, for example dairy and beef farms.
- Comprehensive nutrient management plans should be mandatory, and Wales are currently seeking nutrient handling actions. This action will contribute to Wales’ efforts to reduce total UK emissions

2.6.2 Northern Ireland (Áine O’Reily, DAERA)

- Northern Ireland currently has high NH_3 emissions from the agriculture sector, and many of their sensitive ecosystems are affected; over 90% of Special Areas of Conservation (SACs) are experiencing pollution levels exceeding the sites’ critical loads for nitrogen deposition.
- An NH_3 action plan is currently under development. DAERA is trying to develop the methodology to look at NH_3 emissions across Northern Ireland as a whole, as well to assess individual plans and applications; this will assist in targeting local reductions as well as supporting strategic mitigation measures.
- There is ongoing consideration for introducing a tool similar to the AERIUS software currently used in the Netherlands for this purpose.
- There is also an ongoing need to improve the modelling covering the Republic of Ireland, as NH_3 emissions are transboundary and emissions originating in the Republic of Ireland are not modelled to the same level of detail as those in Northern Ireland.

2.6.3 Scotland (Sue Marrs, SNH)

- Nitrogen deposition levels in Scotland are generally not as high as elsewhere in the UK, although there are hotspots where deposition levels are an issue.
- There is an emphasis on understanding where different sources of nitrogen are originating and where those emissions are impacting on sensitive ecosystems. The focus is on a risk-based approach, likely focusing on the hotspot areas. Funding is limited as nitrogen deposition and impacts on sensitive sites is not considered to be pressing in Scotland.
- There is also a keen interest in preserving the integrity of sensitive sites that are not currently damaged by air pollution impacts, as it is recognized that recovery and restoration of damaged habitats is slow and expensive.

3 Summary, evidence gaps and recommendations

3.1 Summary

Current modelling capabilities in the UK can be described as multi-pollutant and multi-impact. The modelling of NH_3 emissions and impacts is arguably some of the most challenging modelling that can be undertaken for several reasons: the emissions are highly spatially and temporally varying (and uncertain), NH_3 undergoes complex chemical reactions in the atmosphere at a wide range of scales, and the impacts include wet and dry deposition and subsequent impacts on ecosystems.

The models available include local scale models such as the suite of ADMS models (scales of up to a few 10s km), empirically-based models such as CBED and full chemical transport models (CTM) such as EMEP4UK, CMAQ and NAME. The UK is well-placed in terms of choice of modelling approach and to some extent, the choice of model depends on the question(s) being asked.

Given the very wide range of temporal and spatial scales over which NH_3 emissions are important, there are arguments for a combined approach of adopting local and regional scale models through model nesting to capture the important processes that take place at a wide range of scales. This modelling approach has for example been adopted by EMEP4UK in modelling London, where the fine detail of London Atmospheric Emissions Inventory (LAEI) sources is nested within the EMEP4UK model. Similar approaches could be investigated for emissions of NH_3.

Taken as a whole, the UK is well-positioned to undertake detailed modelling of NH_3 emissions at a range of scales. The ‘process-based’ models such as CMAQ and EMEP4UK are particularly attractive in that they explicitly model the important physical and chemical processes leading to a wide range of ecosystem impacts. On the other hand, empirically-based models such as FRAME (as used in UKIAM) potentially offer faster, pragmatic tools for policy evaluation and the consideration of interventions and local (sub 1km) emission sources and receptors. As such, in order to determine the appropriate modelling tool to address a particular policy question, the optimum balance between the additional modelling time and effort required to produce more detailed results, and the need for rapid policy evaluation, should be established.

Learning can be shared between modelling approaches and should be explored for predicting effects of ammonia on ecosystems. For example, in terms of source apportionment and predicting changes in deposition (and indeed other impacts) associated with specific interventions, some models can ‘tag’ emissions. This process allows for the fate of specific emissions to be understood in terms of their emission sources through to their final contribution to an impact. These types of approaches have been used extensively in the modelling of tropospheric ozone but have not, to our knowledge, been applied to the modelling of wet and dry deposition.

It is clear that the appropriateness of the UK NH_3 emissions inventory is of importance to all models. Ideally, modellers need highly spatially and temporally disaggregated emissions to properly capture the dispersion, chemical reaction, deposition and fate of NH_3 emissions in a robust way. NH_3 is difficult to model because the emissions can be diffuse, transient and fugitive. The NH_3 inventory – similar to the rest of the NAEI – is focused on providing information for international reporting rather than as input to air quality models. Emissions of NH_3 depend on factors such as ambient temperature and humidity. The question was raised as to why the emissions inventory assumes fixed meteorology for ambient temperature effects instead of coupling the emissions to the climatology relevant for a specific year. Modellers expressed a preference for an inventory that could respond to climate effects and which was not ‘baked in’. Such an approach would allow modellers more control over adjusting the emissions in response to ambient temperature and other factors. Recent improvements in the inventory, for example in relation to livestock numbers, could be used to improve model accuracy. Improvements both in temporal and geographic resolution as a result of using British Cattle Movement Service Data offer an improved activity data for baseline emissions. In contrast to inventory-based needs, a greater driver for improvement of NH3 emission source detail could be establishment of accurate air quality baselines for decision-making related to local effects on protected habitats and wildlife.

The workshop attendees provided some detailed information on their models but there was little specific information on the analysis of interventions to control NH_3 emissions and impacts on ecosystems. While a model intercomparison of deposition models has previously been carried out for Defra, the evaluation did not consider the effects of various interventions to test model response (Dore, et al. 2015). Based on the wide range of modelling approaches available (local to global, empirical to full CTM), it is likely that the models would show potentially important differences in the way they respond to NH_3 reduction interventions. For this reason, a model intercomparison exercise focused on understanding the response of models to changes in NH_3 emissions would be highly valuable.

Related to the evaluation of models is the availability of ambient measurements of NH_3. It was noted that some of the locations where measurements are made are prone to local issues making it difficult for models to use such data. Furthermore, there are only two locations where hourly measurements of NH_3 are available (Chilbolton and Auchencorth), which is also a limitation from a model evaluation perspective.

In terms of future research needs, the role played by amines was mentioned. The emission of amines is thought to contribute significantly to the formation of aerosols that cannot be explained by SO_2 and NH_3 alone (Almeida, et al. 2013). These processes are currently not accounted for in atmospheric models but recent research in this area suggests it will be important to look beyond the impact of NH_3. Agricultural emissions are thought to be an important source of amines and in particular methylamines (Sintermann and Neftel 2015).

3.2 Evidence gaps and recommendations

Based on the discussions that took place during the workshop, the following is a list of recommendations focused on improving the understanding of NH_3 emissions and concentrations, and addressing current evidence gaps.

- There is a need to consider the development of the NH_3 emissions inventory in more detail from the perspective of use in air quality models, in terms of increasing the level of detail with regards to spatial and temporal variability of emissions. Increased detail of spatial variability i.e. at a farm level would allow improved understanding of local baseline emissions and concentrations, and would assist in targeting mitigation measures to areas where NH_3 emissions occur in close proximity to sensitive sites. This would also facilitate model nesting, i.e. of a local model nested within a national model, allowing for different levels of analysis detail. Increased detail of temporal variability would be useful because emissions of NH_3 depend on factors such as ambient temperature and humidity. The current version of the UK Agriculture GHG and Ammonia Emissions Inventory offers some improvements to spatial (10 km grid cells) and temporal (monthly) resolution, as compared to the previously used national-scale NARSES model (Webb and Misselbrook 2004). However, as discussed in Section 2.4.2, the meteorological data used in the inventory is based on a fixed 30-year period from 1981 to 2010. It should be noted that using climate data in this way is best practice for inventory development rather than using single year weather data. There was specific interest from the workshop attendees in developing an NH_3 emissions model that can respond to factors such as changes in climate, which would allow modellers to match model meteorological data with emissions data that responds consistently with climatic variables.

- A further driver for improving the detail on NH_3 emissions is to produce more accurate air quality baselines and mechanisms to assess new emission sources near sensitive ecosystems.
- Because the impacts of NH_3 are relevant from the small scale (e.g. farm / field level) to regional (continental-scale) there are arguments for retaining several approaches to air quality modelling including empirically-based models, and local to regional models. The impacts to ecosystems are the result of complex chemical processing in the atmosphere. For this reason, 'process-based' full chemical transport models have an important role in capturing the complexity of NH_3 emissions and concentrations where this is required to answer the policy question.
- All the modelling systems discussed in the workshop have the capability of assessing interventions e.g. to NH_3 emissions mitigation at some scale. However, there has to date been no consistent model evaluation exercise conducted to assess the response of these models to interventions. Experience in other modelling domains, including urban and regional ozone models, suggests model responses to interventions are likely to vary widely depending on the model itself, the model set up and the quality and availability of good emissions inventory data. The careful design and execution of a model evaluation exercise would be highly valuable in providing key information on the likely impacts of NH_3 mitigation, and will elaborate on the strengths and weaknesses of the various modelling systems currently available. This would address some of the specific objectives set out in Section 1.2, such as estimating uncertainty and limitations of calibration between models, which are difficult to address without carrying out a modelling intercomparison study.
- It is clear that the topic of NH_3 mitigation cuts across many environmental policy areas – more so than other air quality modelling activities. There are clearly wide-ranging needs from modelling activities, and it will be important to include these wide interests in modelling activities that aim to consider the impacts of mitigation.
- The validation of models against measurements is an important activity. There are a limited number of monitoring sites which monitor NH_3 concentrations in the UK, and there is also a lack of highly temporally resolved NH_3 concentration measurements in the UK (i.e. at hourly time scales). An increase in the availability of such data would potentially help improve both emission inventory verification and the quality NH_3 modelling tools.
- While the focus of NH_3 mitigation is on ecosystem impacts, the role that NH_3 plays in the formation of $PM_{2.5}$ is also very important. Indeed, recent air quality modelling suggests reducing NH_3 emissions can be more effective than reducing the emissions of primary $PM_{2.5}$ in terms of reducing exposures to particulate air pollution (Air Quality Expert Group 2013). It will be important therefore to consider the effects of NH_3 on $PM_{2.5}$ concentrations, in addition to the impacts that NH_3 has on ecosystems.
- Defra should retain a watching brief on emerging issues such as the emission of amines and interaction between many small emission sources, which may well have an important role to play in the emissions from agricultural activities and effects on ecosystems.

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Appendix 1 – Workshop details

Location: Ricardo Energy & Environment, 30 Eastbourne Terrace, London W2 6LA

Date: Wednesday 30 January 2019

Table 2: Organisations and individuals in attendance

Organisation	Name
CEH (Centre for Ecology & Hydrology)	Laurence Jones
CEH (Centre for Ecology & Hydrology)	Mark Sutton
CEH (Centre for Ecology & Hydrology)	Massimo Vieno
CERC (Cambridge Environmental Research Consultants)	Catheryn Price
Creedy Associates	John Morgan
DAERA (Department of Agriculture, Environment and Rural Affairs)	Aine O'Reilly
DAERA (Department of Agriculture, Environment and Rural Affairs)	Charlotte Stewart
Defra (Department for Environment, Food & Rural Affairs)	Ailsa Stroud
Defra (Department for Environment, Food & Rural Affairs)	Jenny Horrocks
Imperial College	Helen ApSimon
Met Office	Matthew Hort
Met Office	Noel Nelson
Natural England	Susan Zappala
Natural Resources Wales	Jiping Shi
Ricardo Energy & Environment	Becky Jenkins
Ricardo Energy & Environment	David Carslaw
Ricardo Energy & Environment	Hugh Martineau
Ricardo Energy & Environment	J Webb
Ricardo Energy & Environment	Jessica Virdo
Rothamsted Research	Tom Misselbrook
Scottish Natural Heritage	Sue Marrs
University of Hertfordshire	Ranjeet Sohki

Table 3: Models represented at the workshop

Model	Full title	Representing Organisation
AQUM	Air Quality in the Unified Model	Met Office
NAME	Numerical Atmospheric-dispersion Modelling Environment	Met Office
CMAQ	Community Multiscale Air Quality Modelling System	University of Hertfordshire
EMEP4UK	European Monitoring and Evaluation Programme 4 UK	CEH
UKIAM	UK Integrated Assessment Model	Imperial College
ADMS	Atmospheric Dispersion Modelling System	CERC
UK Agriculture GHG and Ammonia Emissions Inventory	UK Agriculture Greenhouse Gas and Ammonia Emissions Inventory	Rothamsted Research/Ricardo

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