21GRD10 – quantiAGREMI

D5: Good Practice Guide on quantification methods and uncertainty for NH3 deposition from livestock housing and tracing nitrogen deposition (e.g.15N) in managed soils.

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Contents

Executive summary

This Guidance has been developed to provide a basic resource for planning assessment of the NH_3 concentration and deposition footprints. It introduces statistical modelling tools which help inform both the design and uncertainty assessment of field experiments to measure the concentration field around an animal housing.

Key points

- Guideline on methods and uncertainty for determining spatial distribution of N deposition in the vicinity of animal housing are essential for planning assessment of the potential impacts of NH_3 deposition on farmland and exposure of sensitive receptors in proximity to the emission source to be assessed.
- NH_3 deposition from farming emissions is frequently assessed primarily through the use of air dispersion models (ADMs).
- It is important that ADMs are set up correctly to represent the situation being considered and are undertaken by experienced consultants. There are considerable resources available currently online with advice to do this.
- Measurement of NH_3 in air close to emission sources is carried out less frequently but can provide validation and verification to modelled data.
- Measurement data can also be used to quantify the NH_3 component of N_{dep} empirically usually in combination with meteorological data and some level of explicit process modelling.
- The applied approach is always constrained by resource, availability of sites, timeframe, and economics.
- Measurement approaches ranging from single-point model validation through to flux measurements are described.
- A matrix of approaches with varying levels of modelling and/or monitoring in terms of spatial and temporal sampling and replication is presented.
- ^{15}N has been investigated as a proxy signal. However, no clear pattern in the $d^{15}N$ signal was observed. More details are given in Deliverable 6 of the quantiAGREMI project.

This Guidance should be used as a starting point to understand the trade-offs in undertaking NH_3 footprint assessments and that statistical tools that now can bring quantification to the extent and uncertainty of the footprint in the context of the complex emission landscape which occur in agricultural regions.

Using tools as introduced here, it can be possible to derive a minimum number of diffusive samplers for a given question and a required uncertainty level. The trade-offs between using one analyser sampling in high temporal resolution and a network of low temporal resolution samplers can be understood and used for planning NH_3 concentration and deposition monitoring.

Readers are referred to the references cites for more detailed descriptions of methods and approaches.

1. Introduction

- The agriculture sector is a major contributor to the emissions of ammonia (NH_3, 93 %) and greenhouse gases (GHG) in the form of nitrous oxide (N_2O, 72 %) and methane (CH_4, 48%) in Europe (EEA, 2020)
- The EU Farm to fork strategy aims to reduce GHG emissions from agriculture and food value chain to 55% compared to 1990 levels by 2030, as well as a reduction in nitrogen (N) losses by at least 50% of which NH_3 is a major component.
- NH_3 is emitted from farming practices including livestock housing, waste storage, anaerobic digestion plants, fertiliser and manure spreading.
- NH_3 gas is not simple to measure – it is "sticky" and interacts with surfaces of materials, it dissolves in water and can be re-emitted. Humans emit NH_3 through skin and breath which increases the potential for sample contamination.
- Assessing NH_3 deposition from animal housing emissions is necessary for determining the effectiveness of mitigation practices, to minimize related environmental and human health risks and maximize nitrogen use efficiency (NUE).
- NH_3 deposited in the nearfield of animal housings adds to applied nutrient N loads (e.g. manure, fertiliser) on agricultural land.
- In semi-natural ecosystems, the NH_3 emissions affect both the air pollution pressures on biodiversity and the nutrient and greenhouse gas emission status of the ecosystem.
- There is a significant knowledge gap regarding methods to quantify the amount and spatial extent of N deposition, particularly NH_3 deposition in the vicinity of animal housings from the housing.
- This guidance is aimed primarily at providing details and considerations to be taken into account when choosing model, measurement technique and model-measurement fusion approaches available for quantifying a NH_3 deposition footprint from an animal housing.

1 Approaches to quantifying NH_3 deposition

Quantifying the NH_3 deposition footprint from a point source, such as livestock housing, can be achieved with a range of approaches (Figure 1). These methods range from a highly parameterised atmospheric dispersion model (ADM) integrated into an on-line screening tool to direct measurements and detailed physical chemistry models to calculate nitrogen deposition (N_{dep}).

Where measurements are employed, NH_3 concentration measurements are combined with parameterisations or model approaches to calculate the NH_3 deposition field. These approaches can be categorised into validation/verification, calibration, or direct measurement, with each category providing different information.

The following sections summarise the model and measurement techniques that are typically used by practitioners to quantify the NH_3 concentration and deposition footprint or impact from animal housing emissions.

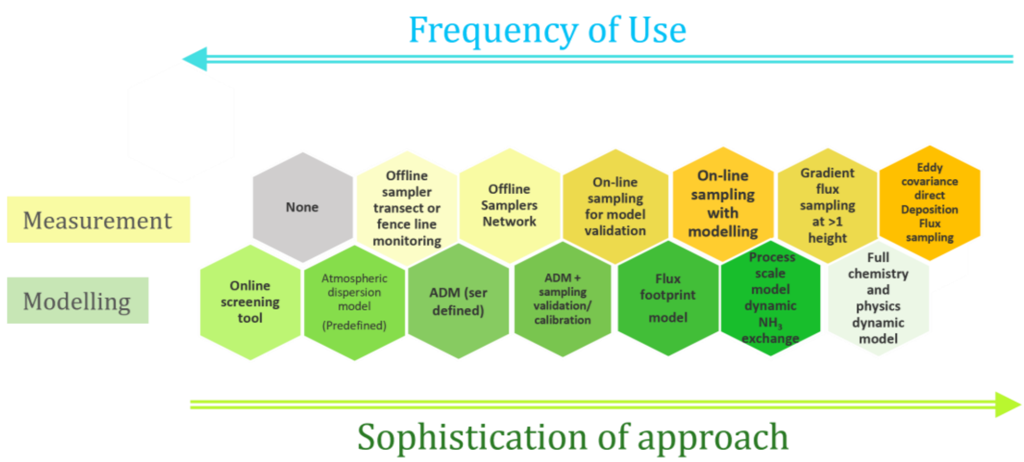


Figure 1 Matrix of approaches used to assess the NH_3 air concentration field and deposition from an emission source.

1.1 Atmospheric Dispersion Modelling (ADM) approaches

NH_3 deposition from animal housing is usually modelled. At the early stage of planning and assessment online screening tools are typically used (refer to Table 1 for examples). These screening tools have ADMs underpinning them, for example SCAIL Agriculture is running the atmospheric dispersion model AERMOD to model NH_3 emissions from livestock installations and associated storage and spreading. But uses offline regional wind statistics for UK and Irish meteorological stations and has other functionalities including directly comparing concentrations against ecological thresholds at sensitive sites. These are designed to be as simple and parameterised as possible and are frequently automated for reasons of cost-effectiveness and efficiency, given the number of agricultural installations which need to be assessed in the planning and regulatory systems. A widely used example of a screening tool is SCAIL, (Simple Calculation of Atmospheric Impact Limits) which is used in the UK and Sweden. UK SCAIL was developed for pre-planning conservative (highest scenario concentrations) checks prior to undertaking detailed modelling or measurements (Theobald et al. 2009).

Short range ADMs are designed to simulate the atmospheric transport and deposition of atmospheric pollutants over relatively small distances, typically from tens of metres up to a few kilometres. These models are typically used to assess the impacts of a point source. Examples of short range ADMs include advanced dispersion model (ADMS), United States EPA AERMOD, Operational Priority Substances (OPS-st) model and Dutch Atmospheric Large-Eddy Simulation model (DALES, Schulte *et al.* 2022). The modelling approaches include Lagrangian stochastic particle models, Gaussian plume dispersion models, Eulerian models, and large eddy simulations (see Loubet et al. 2009 for further details). ADMS and AERMOD are examples of Gaussian plume models, which calculate the concentration or deposition field, often for a single emission source, and take into account the vertical profile of the boundary layer parameters (Loubet et al., 2009, Theobald et al., 2012). A more complex implementation of an ADM is a multisource model, an example being the Landscape Area Dispersion and Deposition Model (Dragosits et al. 2002; Vogt et al., 2013). It incorporates land cover class, specific dispersion, and deposition characteristics, as well as meteorology to predict concentrations and deposition of NH_3 across a landscape with multiple agricultural NH_3 sources.

ADM approaches, highlighted above, require significant background information (e.g. source characteristics, meteorological information, receptor information) to inform the model. The ADMs listed operate with a mix of pre-selected conditions and user defined input data. For example, meteorology can either be modelled or measured, as well as user defined emission factors or deposition parameterisation. Table 2 summarises the typical set of input parameters required for an ADM.

Given the general nature of the parameters in Table 2, once detailed N deposition modelling is required, the inputs to the model can be made locally/source specific. For example, the emission strength can be modified from a standard emission factor if a different management approach is used compared to the reference, or local meteorology measured at the point of emissions can improve the modelling of the spatial characteristics of the NH_3 footprint.

Table 1 NH_3 deposition modelling approaches without measurements (Note: arrow means e.g. unidirectional/bi-directional)

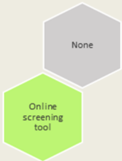
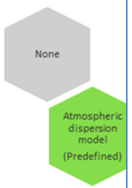
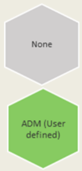
Model approaches/ model)	Emission	NH_3 Chemistry	Met	NH_3 Deposition v_d	Detail	Use	Advantages	Challenges	Typical uncertainty	References
	Set emission factors for housing type	None	Parameterised, e.g. typical met year for location	↓	Simplified ADM interface underpinned by basic/standard? background ADM	Early-stage assessment of new N_{dep} source in agricultural landscape	Simple to use. Regulator and industry useable outputs	N_{dep} at points only rather than footprint	High, used for conservative screening at planning stage	Hill et al. 2014
	Set or user defined for housing type	None	Parameterised or local measured	↓	Commercial and free models with simple Gaussian dispersion	Plume modelling for air concentration and deposition	Off-the-shelf Consistent and comparable for regulators and planners	Higher uncertainty due to local factors, air and surface chemistry not included	Medium-High: Function of model setup;	
	Set or user defined for housing type	None	Local measured	↓	As above but using experts to set up model with local parameters e.g. met, housing	Detailed modelling for a specific installation and scenarios	Still off the shelf but tailored to allow best outputs possible.	User-input parameters possible but not widely used		
	Set up by user	Can include gas phase & aerosol reactions Plant surfaces	From parameterised through to detailed fluid dynamic modelling	Surface specific from literature ↕	e.g. landscape models, bespoke R based "big leaf" models, nested chemical transport models	Detailed impact assessment and chemical pathway sciences	State of the art. User needs to be an expert.	Not widely available or tested	Validation of models not widely undertaken; uncertainty unknown but likely low	Ge et al. (2022); Deshpande et al (2024)

Table 2 Summary of typical information and parameters for an air dispersion modelling (ADM) approach to measuring NH_3 air concentrations and deposition.

Category of information	Detail
Assessment information	Emission source to be modelled
Assessment information	Details of the modelling software
Assessment information	Criteria/purpose of the modelling
Assessment information	Details of source input data
Model inputs	Emission sources in model domain
Model inputs	Animal number/type in each emission source
Model inputs	Housing ventilation details
Model inputs	Land spreading details (if relevant)
Model inputs	Emission factors used from literature
Model inputs	Baseline data for background concentrations
Model inputs	Meteorological data and method used (modelled or measured)
Model inputs	Terrain
Receptors	Human habitations
Receptors	Habitats and sensitive features
Receptors	In-combination effects (if doing a planning assessment)
Receptors	Surface roughness
Receptors	Deposition velocity/parameterisations used
Receptors	Air quality or knowledge aims relevant for the modelling exercise
Results	Modelling period
Results	Model output data
Results	Average NH_3 in air (e.g. either for modelling time period or annual average)
Results	Site location map
Results	NH_3 deposition
Results	N_{dep} change due to modelled emission source (Note: this can be set up to separate dry gaseous, aerosol and wet deposition components)

1.1 NH_3 measurement and modelling approaches.

NH_3 concentration measurements, in proximity to animal housing, can be used for many purposes including to assess the performance of models (verification/validation), to calibrate model output or to be used directly to monitor air concentrations of NH_3. With sufficient resources, NH_3 measurements may be taken with sufficient resolution to derive a NH_3 concentration field across the footprint of the animal housing. Atmospheric NH_3 concentrations are spatially skewed, decreasing exponentially with distance from emission source due to dispersion (e.g. Loubet et al. 2009, Bell et al. 2016,). For suitable ADM validation, datasets must consist of measurements made using a reliable and accurate method – with uncertainties specified. Measurements must be made in locations and conditions relevant to model or tool which is being validated.

NH_3 can be measured with on-line analysers that measure NH_3 directly at high temporal resolution ~seconds-mins) or off-line sampling approaches which sample the air over a period of time (~days-month) and the sample is then analysed in a laboratory to produce a total concentration for the period. Both these types of measurement are briefly discussed here but other reviews cover measurement techniques in more detail e.g. Twigg et al. (2022) and Braban et al. (2018).

The on-line high-resolution NH_3 concentration analyser technology market has been rapidly developing in the early 21st century and recent studies have assessed analysers available (e.g. Pogany et al., 2016, Twigg et al., 2022). Typically, on-line analysers can be open path systems such as the mini-Differential Optical Absorption Spectrometer (mini-DOAS, Bell et al. 2017) or closed path analysers such as cavity ring-down systems and quantum cascade laser absorption spectrometers (Twigg et al. 2022). Until recently, closed path systems have been favoured due to their development for the commercial market and relative ease of use and are "plug and play" technologies, though care needs to be taken with all types of analysers to make sure contamination internally or on surfaces of open path systems are prevented or accounted for in the quality assurance of data. The challenges are due to the sticky nature of NH_3 interacting with any surface, water, and particulate matter in air. Inlet designs and analysing system maintenance and QAQC is essential for collecting accurate NH_3 data. This issue is discussed in detail in Twigg et al. (2022). There are also several on-line wet chemistry approaches, which are state-of-the-art but require high labour inputs.

Off-line sampling approaches sample by accumulating air on a media which is then extracted into ammonium (NH_4^+) and analysed offline with wet chemistry approaches. The concentration is then calculated back to NH_3 using the measured volume of air or applying a rate of uptake onto the media based on the length of exposure. Diffuse or slow sampling active samplers have a sampling period ranging from 1- 4 weeks, but exposure times are dependent on the concentration range and detection limits of the method (refer to EN 17346:2020 for further details).

Measurement assessments for NH_3 concentrations or fluxes with a view to deriving N-deposition with a model usually cover short periods around agricultural housing and great care should be taken extrapolating to annual average NH_3 concentrations and N-deposition. Figure 2 illustrates the ways in which a concentration field or footprint/footprint section can be assessed with measurements and basic considerations for each type of approach which comprises of measurement and modelling in Figure 1**Error! Reference source not found.** and are summarised in Table 3 and Table 4. The matrix of approaches with varying levels of modelling and/or monitoring in terms of spatial and temporal sampling should be used as a guide for the approach that is relevant and appropriate for applications and evidence needs.

The spatial extent of the footprint from an NH_3 emission source can be <1 km up to many kms depending on the strength and height of the emission source, topography, and meteorology. For small sources, the full footprint (Figure 2 (1)) can be measured with flux measurements but more frequently, only part of the flux footprint is assessed (Figure 2 (2)). The flux measurement location is an expert scientist level decision as there are complex and specific criteria such as local meteorology, topography and footprint representativeness which can influence the measurements.

Where NH_3 flux measurements are not possible, on-line NH_3 concentration and meteorological measurements can be used to drive models such as backwards Lagrangian Stochastic Model (b-LM) to calculate emissions and/or deposition. B-LM approaches can assess all or a fraction the NH_3 emission source footprint. (Figure 2 (3) and (4)). See Kemp et al. (2021), Hani et al. (2018) and references therein for more detail. Similar to flux measurements, for concentration monitoring, the measurement location is an expert scientist level decision as there are complex and specific criteria which influence the decision. These factors include local meteorology, footprint representativeness of vegetation/surface, topography, building infrastructures, access to mains power. Models such as Windtrax (see Tagliaferri et al. 2023 and references therein) and the Kljun footprint models (Kljun et al. 2015) have been used for these types of studies as well as bespoke models developed in research groups, which require expert scientist input.

Remote sensing either from satellite (Clarisse et al. 2010) or with airborne systems (Camarillo-Escobedo et al. 2022, Noppen et al. 2023) which assesses the whole footprint of an animal housing **Error! Reference source not found.** (5)) has been used for research on NH_3 concentrations in ambient air and the plumes from animal housing. At this time, satellite remote sensing has limited resolution such that to assess individual sources would require long term averaging and careful data handling and would currently primarily be applicable to large scale farming or industrial emission sources rather than assessment of individual housing. There are also challenges with issues with interferences and discriminating the near-surface concentrations. Though it is likely in the future this measurement ambition will become achievable at present there is no remote sensing approach which will allow NH_3 concentration fields and N-deposition footprints to be routinely quantified.

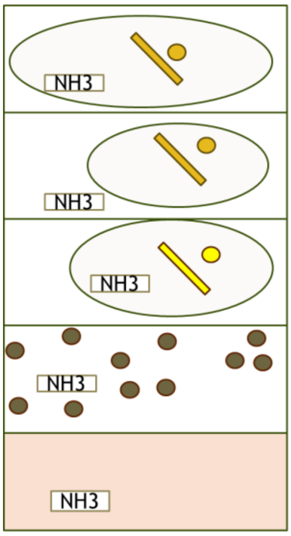
In the majority of studies and assessments, the NH_3 footprint around an animal housing is assessed with a network of off-line NH_3 samplers and concentration sampling, transect decay curves or spatial assessments designed and monitored, for a short period of time or across a housing cycle or season/year. The number of samplers is constrained by resource, availability of sites, timeframe and economics. NH_3 sensors, which report at higher temporal resolution, are beginning to be available at very near-source NH_3 concentration levels (>>10 $\mu g.m^{-3}$) however there is very little qualitative or quantitative assurance on the performance of these sensors in the field.

Uncertainty in on-line high-resolution analysers range from 3 to 10% (Erisman, 2001; Norman et al., 2009), with accuracy decreasing when the sampling system becomes contaminated with NH_3, particulate matter or is affected by temperature cycling. Uncertainty for passive diffusion samplers such as active denuders, diffusion tubes has been estimated between 15% (Twigg et al., 2022) to

39% (Leiva G. et al., 2013), again with the caveat that system cleanliness and quality assurance best practice is needed to ensure quantitative measurements are possible.

Beyond the analytical uncertainty of the measurement, there is less information regarding uncertainty and best practice for monitoring design for NH_3 around animal housing, though a wide range of design and representativeness assessments of monitoring air pollutants have been used in other studies (see Raine et al. 2024 and references therein)

This document is a first guidance on designing a NH_3 monitoring network around an ammonia source (Figure 2 (4)) and quantifying uncertainty systematically. This Guidance is based on a desk study and literature review, and data from measurement campaigns and presents information to steer future studies which address the challenge of design a deployment of off-line samplers (Section 3). From this, simple, high-level suggestions are made for those planning future studies (Section 4).



1	Flux of whole source footprint	NH_3 Deposition	Capital & Operations costs high	Uncertainties can be calculated explicitly	Limited expertise base
2	Flux for part of housing footprint.	NH_3 deposition and extrapolate	Capital & Operations costs high	Uncertainties can be calculated and extrapolated	Limited expertise base
3	High resolution concentration all or part of footprint	NH_3 concentration	Capital & Operational costs medium	Uncertainties can be calculated and extrapolated	Moderate expertise base
4	Low resolution concentration all/part of housing footprint	NH_3 concentration	Low capital costs; Operational costs medium	Uncertainties can be calculated and extrapolated	Moderate expertise base
5	Whole farm remote sensing/ satellite	NH_3 column	Low but limited control of product	Uncertainty in remote sensing knowledge required	Limited expertise base

Figure 2 Summary of measurement approaches to understand NH_3 concentrations and surface deposition near animal housing.

Table 3 Combined Measurement and Modelling approaches available for NH_3 concentration and deposition measurement.

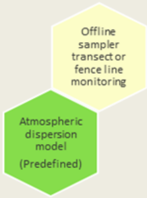
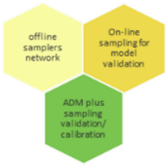
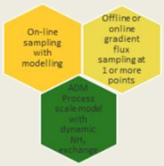
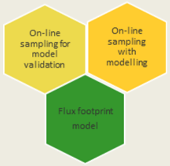
Measurement/ model mix	Emissions	Chemistry	Physics	V_d	Measurement Detail	Use	Advantages/ disadvantages	Measurement requirements	Example Reference(s)
	Set emission factors for housing type	None	Set dispersion and modelled meteorology for location	↓	Measurement data to validate or calibrate at 1 or more points in proximity to emission source	Modelling validation in actual location, usually undertaken when model results are close to or above thresholds	Relatively inexpensive ✓No power ✓No expert field work ✓Diffusive sampling standard available EN 17346 (2020) × No temporal information × Expert experiment design needed	► Over the relevant housing emission cycle up to 1 year. ►Time: ideally monitoring should be length of housing cycle or 1 year ► Expert experiment design ► Access to laboratory capability	Hill et al. (2014)
	Set or user bespoke emission factors for housing type	None	Set dispersion and can use measured local meteorology	↓ or ↕	Offline data can be used to assess spatial NH_3 distribution. On-line instrument can be used to study temporal NH_3 distribution and be used for modelling/independent test of ADM	Assessment of Emission and deposition with independent parameters to identify aspects of emissions which may be outside model (e.g. concentration spikes)	Moderately expensive ✓diffusive sampling standard available EN 17346 (2020) ✓ spatial & temporal data ✓ local meteorology ×Expert design ×Access to laboratory and field capability	► Power for on-line instruments ► Expert field technicians ► Needs to be over the relevant housing emission cycle up to 1 year. ►Time: ideally monitoring should be length of housing cycle or 1 year ► Expert experiment design ► Access to laboratory capability	Miller et al. (2015) Bell et al. (2016)
	Measured or set emission factors	Basic NH_3 reactions	Measured 3D meteorology to allow stability constants and turbulence to be used	↕	Offline and on-line data can be used to parameterise the concentration field and deposition model	Identify the fate and lifetime of NH_3 in the area of the footprint; quantify the magnitude and extent of the NH_3 footprint	✓ Spatio temporal concentration and deposition dataset × Expensive × Expertise	► Power for online and offline gradient sampling ► Expert field technicians ► Needs to be over the relevant housing emission cycle up to 1 year. ►Time: ideally monitoring should be length of housing cycle or 1 year ► Expert design ► Expert modellers	Deshpande et al. (2024)

Table 4 Measurement and modelling approaches using NH_3 flux measurements.

Measurement/ model mix	Emissions	Chemistry	Physics	v_d	Measurement Detail	Use	Advantages/Disadvantages	Measurement requirements	Example Reference(s)
	Not required method is a direct measurement of emission and concentration field	None	Directly measured meteorology parameters required. Data used to calculate atmospheric stability constants and turbulence.	↓ or ↕	Measurement-model fusion approach. Offline and on-line concentration vertical profile data used to inform the modelling of the deposition field.	Calculation of emissions or deposition rates	✓Best available method for quantifying deposition or emissions ˣcapital investment large ˣexpertise and tine investment large ˣchallenging as need very specific conditions to get best data	Mains power required typically. ► expert experiment design ► expert field technicians ► homogenous flux footprint required limiting the application near point sources	Swart et al. (2021) Sun et al. (2015)
	Not required as method is a direct measurement	Not applicable: direct measurement of flux, so no chemistry correction required.	Instantaneous measurement of turbulence and NH_3, to derive a flux.	↕	Provides process understanding of the drivers of deposition and emission of NH_3. Parameterisations for ADM is derived from this approach.	Deposition process parameter measurement; model testing; Net deposition/ emission	✓Direct measurement of deposition (where applicable) ✓ High temporal concentration and flux dataset (both emission and deposition) ˣ Expensive ˣApplication limited near to livestock buildings due to advection errors.	► Mains power required typically ►Capital investment large ►High instrument reporting resolution required (>10 Hz typically) ►Expert experiment design ► Expert field technicians ► Homogenous flux footprint required limiting the application near point sources	Mauder et al., (2021), Whitehead et al. (2008).

2. Considerations for designing NH_3 footprint measurement using sampler/sensor network.

The spatial representativeness of monitoring stations/sites is important for network design and optimisation and is discussed in detail in Raine et al. (2024). Key questions which need to be understood are:

> *How does the uncertainty in the estimated NH_3 concentration field change with varying numbers of monitors around a typical emission source?*
> *How many sensors are needed to quantify the NH_3 concentration field around a typical emission source to have a pre-specified uncertainty?*

Deriving answers for these questions will enable logistics and financial budget decisions to be taken with confidence. This Guidance focusses on the deposition footprint on an animal housing, however it is emphasised that there are other purposes for NH_3 measurements, and for those there are different monitoring requirements depending on circumstances. For example, in some cases to assess NH_3 impact on nature at one specific location, the emission source concentration field is not required, but monitoring focusses at the closest edges of sensitive habitat receptors. In other applications, samplers can be deployed to verify contributions from a permitted emission site regulatory purposes either using a very a low-density network or set of sites (SEPA, 2018).

Spatiotemporal models can provide an enhanced method of estimating the concentration field by integrating monitoring network that can improve the ability to determine the spatial covariance structures. Using statistical approaches to model ammonia concentration from monitoring station data allows for more explicit incorporation of variability into modelled outputs. In the case where the concentration and deposition footprint are aims of the monitoring (e.g. to model from measurement the NH_3 concentration field from an emission source), to ensure a statistically rigorous definition of the spatial representativeness area around a single monitoring station, the following would need to be considered and accounted for:

- The area surrounding a monitoring site at which the pollutant concentration is estimated to be statistically equivalent to the concentration observed at the monitoring station.
- This concentration measured is within the detectable operational range of the sampler.
- The uncertainty of the sampler equipment, between sampler replicates and in the modelled concentration field are quantified.
- If an estimation of the spatial representativeness of a monitoring station across an entire monitoring campaign/agricultural activity cycle is being assessed, then this must also take into account variability in pollutant concentrations over time.

- How far from a source can a sensor or passive sampler still detect NH_3 concentration changes above regional background?

High variability in NH_3 concentration in space or time can limit the size of the representativeness area of one monitoring station. The presence of multiple sources of NH_3 that have not been sampled with a sufficiently dense monitoring network to allow for a quantitative assessment of deposition can also affect the uncertainty in estimating an NH_3 deposition field. If the goal of a project is to design a monitoring network to have a low uncertainty across the area surrounding one emission source, then monitoring designs need to more explicitly account for other background sources of NH_3. These other NH_3 sources can be themselves large and can have substantial effects on both the estimated deposition and uncertainties in a modelled concentration field. Through the modelling and discussions with authors of literature studies, it has been ascertained that the design of a monitoring network needs to consider purpose of the exercise, e.g. validation of model, measurement of absolute concentrations, ecosystem protection or emission source discrimination. The design can be done primarily through logistics planning – as often that is the major decision point in planning a campaign, but standards will be better when monitoring design is done in combination with a planned uncertainty and data quality objective.

When designing a field monitoring study, the following criteria and boundary conditions need to be considered:

- Complexity of emission landscape and if the source of interest can be sufficiently isolated from other emission sources in the landscape.
- Complexity of the meteorology, geography and topography and whether the model can take this into account.
- The agricultural cycle of the animal housing and ensuring the monitoring sufficiently captures the temporal change of emissions over the cycle.
- The season of the monitoring and whether the monitoring sufficiently captures the temporal change of the emissions over the annual seasonal cycle and if the interannual changes are likely to be similar.
- The local landscape background and variations through the agricultural calendar.
- The acceptable uncertainty at the edges of the footprint of the animal housing emissions (e.g. credible level and Root Mean Squared error (RMSE)) which will allow modelling to be undertaken or verified.
- Acceptable levels of uncertainty in proximity to the emissions in the footprint of the animal housing emissions (e.g. credible level and RMSE) required to support model development or validation.
- Considering the above criteria and taking into account the available resources and financial budget, design the optimal NH_3 deposition measurement study.

In some studies data is used, rather than a process-based model to map an NH_3 concentration field. Walker et al., (2014) for example, used a non-linear regression model to predict the NH_3 concentration field from a poultry shed, incorporating air chemistry, meteorology, foliage, and soil conditions. Though this approach can provide valuable insight into to the concentration footprint, some studies do not incorporate the uncertainty from the NH_3 monitoring network, even though this can have a substantial impact on the outcomes of the models.

As generally the uncertainty is not currently accounted for in NH_3 modelled concentration fields, studies assumes that the pollutant concentration in a region around the monitoring point does not differ from the concentration measured at the monitoring point. This overlooks that fact that there is uncertainty in these measurements that needs to be quantified and integrated into the workflow for estimating NH_3 emission through to deposition.

NH_3 measurement studies in animal housing footprints assessed in the desk study of Raine et al. (2024) are detailed in Table 5. The approach/applicability for spatial modelling and uncertainty assessment for these measurement studies were reviewed. Appendix A summarises the case studies undertaken with the Bell et al. (2016) and Hill et al (2014) datasets. From this a case study at a farm in the Netherlands was designed to assess and deliver the Guidance in this document.

Table 5 Literature studies monitoring NH_3 concentration fields from agricultural sources.

REFERENCE	SCALE	EMISSION SOURCE	LOCATION	DATA TYPE	DURATION
VOGT ET AL., (2013)	Landscape (5km x 5km)	2 main poultry farms + others across landscape	Scotland	31 passive samplers Model outputs	19 months
SOUHAR (2021)	Landscape	18 livestock houses across landscape	France	28 passive samplers	12 months
BELL ET AL., (2016)	Small: <600m	Anaerobic Digestion (AD) plant	Scotland	20 passive samplers 1 continuous capture	2 months
WALKER ET AL., (2014)	ALPHA: 0.8 - 3.5km, continuous = 10km	Poultry farm	USA	30 passive samplers 1 continuous sampler	24 months
HILL ET AL (2014) WHITELEES	Small: 1km	Poultry farm	Scotland	9 passive samplers: summary data 1 continuous sampler	3 months
HILL ET AL (2014) SCAIL: GLENDEVON	Small: 1km	Poultry farm	Scotland	9 passive samplers	3 months
CAROZZI (2013)	600m	Manure spreading	Italy	2 passive samplers	?

2.1 Bayesian kriging models: understanding uncertainty with spatial NH_3 sampling.

Bayesian kriging models with diffusive NH_3 sampling can be used to isolate the uncertainty associated to the spatial and temporal elements of the NH_3 monitoring network, as well as the uncertainty associated with specific explanatory variables. A Bayesian spatiotemporal model accounts for temporal correlation as well as spatial correlation (typically with closer time points being more similar than distant ones) – essentially, this allows sharing of information between sample periods and can therefore incorporate both the spatial variability in NH_3 concentration, as well as the repeated data points over time that give important information on the temporal distribution of NH_3. Spatiotemporal models can provide an improved method of estimating the concentration field by incorporating more data from the monitoring network that can improve the ability to determine the spatial covariance structures.

In geostatistical analysis, the first stage in classical kriging is to identify the spatial covariance across the dataset, and this is done by fitting a variogram to the pairwise spatial correlations. With limited data points in a monitoring network, it can be difficult to determine the best choice of variogram model and to achieve a good fit for estimating the variogram parameters (where these parameters describe the nature of the spatial covariance). The second stage of analysis uses this spatial covariance structure to provide weightings in a regression-type interpolation, which predicts across the map domain. The approach assumes that the spatial covariance parameters were estimated without error, which is clearly not the case, so gives an unreliable estimate of the total uncertainty. These issues can be addressed using Bayesian approaches. In brief, a Bayesian analysis of geostatistical data enables both the spatial variance information and the interpolation process to be modelled simultaneously (Cressie & Wikle, 2015). Bayesian kriging generates a distribution of possible maps given (a) the measurement data and (b) a number of assumptions on the distribution of parameters that are included as priors. The uncertainty from the mapping process is derived from the distribution of possible maps, so represents uncertainty from both the determination of the spatial covariance structure and the interpolation procedure.

The Bayesian analyses in this study use the R package *inlabru* (Bachl et al., 2019) which provides convenient wrapper functions which simplify the application of R-INLA package (Integrated Nested Laplace Approximation; Lindgren & Rue, 2015). INLA has proven to be a fast and robust alternative to Markov chain Monte Carlo (MCMC) for fitting latent Gaussian models.

A number of correlation functions are commonly used in geostatistics to model association amongst points in space. Here a Matérn correlation is used, with two hyperparameters to estimate (range and sigma – which describe the shape of the correlation function). Priors must be set on these hyperparameters (the distribution of values that we believe the true hyperparameters sit within). From this, a generalised random forest GRF is modelled from which it is possible to make predictions across the concentration field using the resolution defined in the mesh. Each grid cell has an associated probability distribution of possible values, from which a mean and measure of variation (such as the credible interval) can be derived. Log NH_3 concentration is used as the response term, modelled as a function of distance from the emission source(s) and a Stochastic Partial Differential Equations (SPDE) model which is a type of mathematical model describing random phenomena in space and time. Together this allows modelling of the spatiotemporal variability in NH_3 concentration.

1.2 Case study of Bayesian kriging around an animal housing to illustrate measurement network design considerations.

A monitoring network was designed around an animal housing in the Netherlands, with a greater number of sites than in the Raine et al. (2024) Desk Study, in order to be able to assess the effect of number of sampling sites on the RMSE curve. The 30 sites have a site as one location with triplicate ALPHA passive samplers. The present study utilised a considerably higher number of monitoring sites than the majority of previous studies, with thirty sites being used in total (Figure 3). Passive samplers from each monitoring site were exchanged approximately once per week over a period of six weeks. In this case study, the modelling simulated experimental monitoring networks with a fewer number of monitoring sites and assessed the impact this has on the modelled NH_3 concentration and uncertainty estimation from the spatiotemporal model. Eight researchers experienced in designing and implementing ammonia monitoring networks were also asked to select 5, 10, 15 and 20 out of the 30 site locations from the project team experimental design (Figure 3) that they would choose if restricted to fewer monitoring stations to best monitor NH_3 concentration in our study landscape. Experts were told the emission source location, prevailing wind direction and the context of the agricultural landscape only. This approach was chosen to ensure the design of monitoring site locations selected for the scenarios best capture NH_3 concentration within the limited number of sites, rather than a random selection which would give an unrealistic experimental design and amplify error. These site selections were used to run eight simulations of selecting subsets of the monitoring sites from the full network of 30. By sequentially including fewer sites in the eight simulations, the effect that site number has on the overall quality of the model fit gives an indication of the optimal number of monitoring sites needed to represent the concentration field.

From each of the model runs, the RMSE was calculated and used as an estimate of the absolute average deviation between the model prediction and the NH_3 concentrations recorded, i.e. an estimate of the average deviation in the modelled NH_3 concentration from the true value. The average model predicted concentration fields (irrespective of time period) and average 95% credible intervals maps for each model simulation were assessed to explore the effect on the predicted ammonia concentration over space.

NH_3 concentrations varied across the monitoring network over the 6 study periods, with per site triplicate averages ranging from 0.62 to 19.62 µg m^{-3}, with a median of 2.31 µg m^{-3}. The NH_3 concentration per site also varied across the monitoring periods, with a median of 3.88 µg m^{-3} in the first monitoring period, which dropped to 0.99 µg m^{-3} in period four, primarily driven by changing meteorological conditions at the location. Figure 4 and 5 shows that concentration decreases as a function of distance from the animal housing, with Figure 5 showing the Bayesian kriged concentration field taking only the animal housing as a determining variable. Figure 6 shows the predicted concentration field independent assessment of the source contribution, independent from emission factors which can then be used as an output to compare against ADM assessments and calculate NH_3 deposition with a model of the user's choice (see Section 3.3)

In the expert design section of this case study, eight experts all chose their preferred sites for scenarios including 5, 10, 15 or 20 monitoring sites. The initial observation is that even expert opinions on site placement (with limited site information) differ, and these differences can therefore have a substantial effect on the representativeness of the collected data and modelled results. This highlights that decision making in field experiments like this need to be recorded and be part of the metadata of the study. Recording, assessing, and improving decision making to achieve less uncertain results is rarely discussed in NH_3 network design but as improvements in uncertainty are sought, this consideration should be integrated into future studies.

The results from this case study confirm the results of the Desk Study by Raine et al. 2024, showing significantly higher uncertainty with fewer monitoring sites, with 30% increase in RMSE in the median NH3 concentration (model domain median value) between 5 sites and 20 monitoring sites. The difference between the maximum and minimum is 60% (+/-). Hence the number of monitoring sites is an important source of uncertainty to consider, particularly where NH_3 concentrations are being assessed across or adjacent to sensitive habitat receptors. Uncertainty increases exponentially with fewer sites and then decreases more slowly between 15- 20 sites (Figure 7).

It is clear that an assessment at the start of a study as to the acceptable level of uncertainty for the purposes of the measurements is essential to ensure the aims of a study are met. For example, if the uncertainty of well-placed 5 sampling sites is acceptable for the purposes of the study, then more samplers are not required to be funded. In contrast, where a less uncertain concentration assessment is required, then investment in a denser network can deliver the result required.

It is noted that in this study, which was in a complex agricultural landscape, it is possible through the measurement network, to isolate the contribution of the animal housing to the measured NH_3 concentrations and to use the relationship with distance from the animal housing to separate the contribution of the animal housing to the ambient NH_3 concentration as a function of distance. This capability is useful for assessing model predicted contributions from individual animal housings in the landscape. With the assumed log concentration distribution, the results can be used to extrapolate to the contribution of the cattle shed to ammonia concentrations at greater distances.

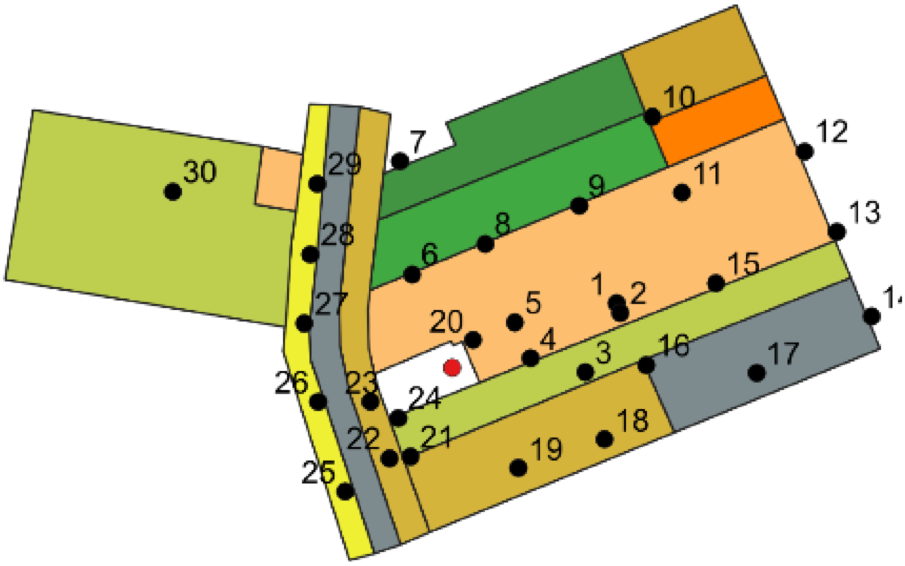


Figure 3 Set up of passive samplers around a Dutch dairy farm (colours show different activities in fields, not specified here)

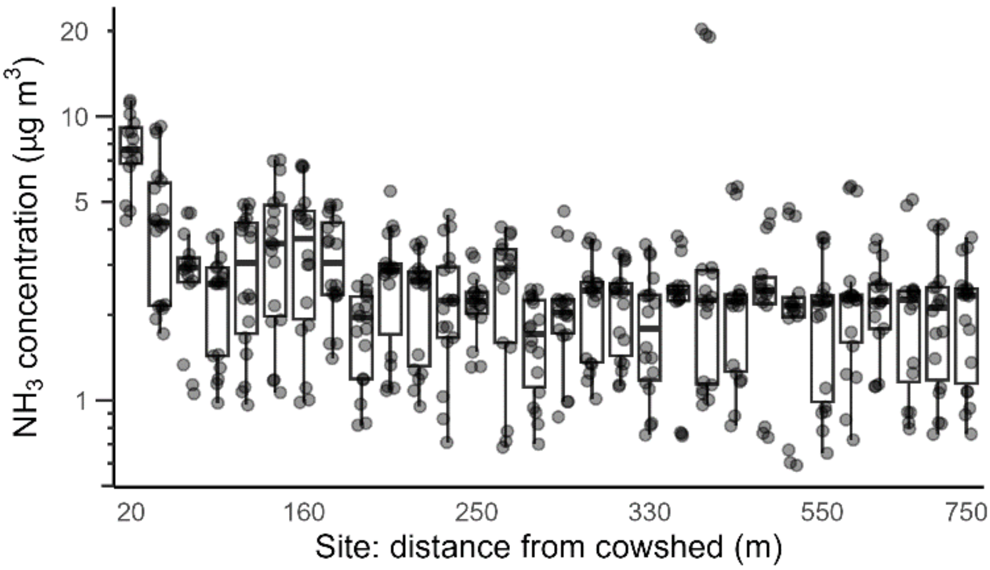


Figure 4 NH_3 concentration as function of distance from livestock building. Boxes show xx, whiskers show yy, points show.

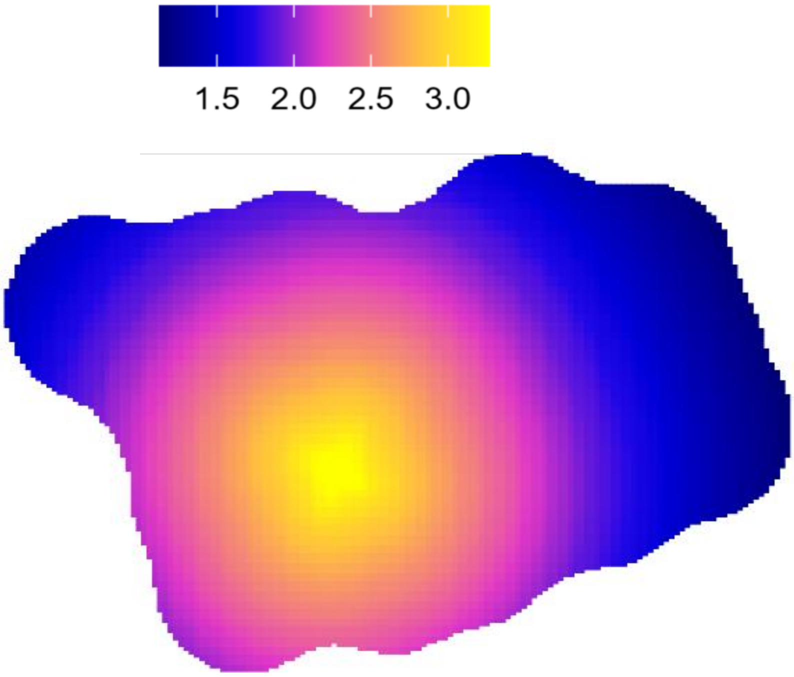


Figure 5 Model predicted median contribution of ammonia concentration (µg m^{-3}) from the animal housing over the modelling domain. The boundary of the domain is ~1.1km from the centre of the emission source.

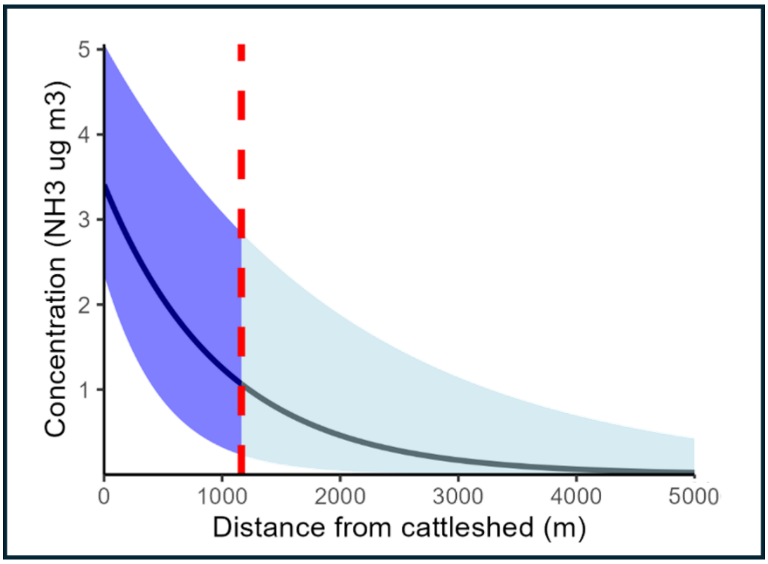


Figure 6 Association between distance from animal housing and ammonia concentration attributed to the animal housing as predicted by the Bayesian model. 95% credible intervals shown by x, the red dashed line indicates x

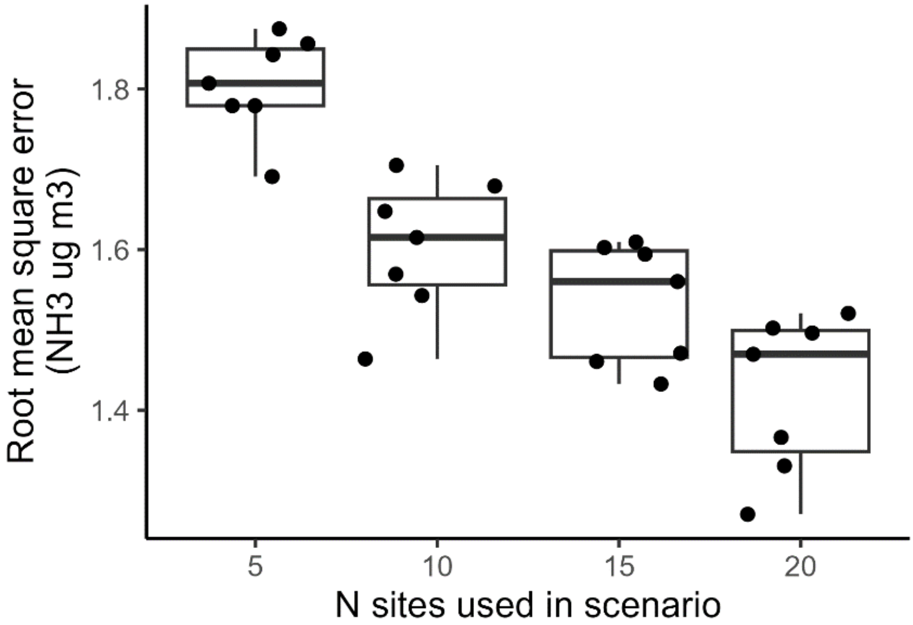


Figure 7 Uncertainty (RMSE) of NH_3 concentration from number of sites selected by experts.

In some studies, quantifying the NH_3 concentration at points or across the animal housing is sufficient of the aims of the monitoring. However, in other studies it is the NH_3 component of the N deposition, which is required to be measured, for example to compare the N deposition from fertiliser application against atmospheric N deposition. Therefore, to progress from a measurement or measurement-driven modelled NH_3 concentration field to NH_3 deposition, a deposition parameterisation needs to be applied. The simplest approach is to use a unidirectional deposition velocity (v_d) is applied to the concentration measurement, irrespective of the vegetation or surface type. This is typically the default setting in many ADMs. In this case study, v_d = 1 cm s^{-1} (Schrader and Brummer. 2014) was used as the single value and for a surface specific approach, each field had a land surface type during the monitoring included as a parameter (Table 6). It is beyond the scope of this case study to detail the explicit differences between the two approaches. However, it is essential to note, that depending on which approach is selected for a study, there are significant differences both spatially and in NH_3 deposition magnitude and this should be considered at an early stage of planning an NH_3 deposition assessment study.

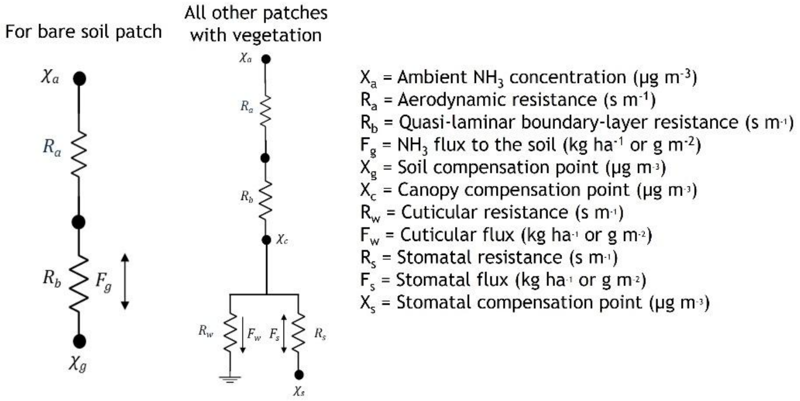


Figure 8 Schematic of NH_3 deposition processes over bare soil and vegetated land.

Table 6 Summary of selected literature gamma (Γ) values for calculating v_d for different land surfaces. Γ represents the dimensionless emission potential (or stomatal compensation point potential) of a surface, such as soil or vegetation

Patch	Land use type	Mean canopy height (m)	Gamma	Reference
1	*Lolium perenne*	0.22 (Periods 1-5), 0.068 (Period 6)	140	Hermann et al., 2009
2	Bare soil	0	14200	Abeed et al., 2023
3	Wheat	0.4	3558	Morgan and Parton, 1989
4	*Lolium perenne*	0.2	140	Hermann et al., 2009
5	Mixed deciduous	15	1162	Deshpande et al. 2024
6	Freshwater	0	NA	V_d of 0.7 cm s^{-1} was used, Schader and Brummer, 2014
7	Grazed mixed grass	0.3	1275	Fowler et al. 2007
8	*Lolium perenne*	0.2	140	Hermann et al., 2009
9	*Medicago sativa*	0.3	233	Dabney and Bouldin, 1990
11	Mixed deciduous	15	1162	Deshpande et al. 2024
12	Maize	0.2	1186	Harper and Sharpe 1995
13	*Lolium perenne*	0.22 (Periods 1-5), 0.068 (Period 6)	140	Hermann et al., 2009
14	*Medicago sativa*	0.3	233	Dabney and Bouldin, 1990

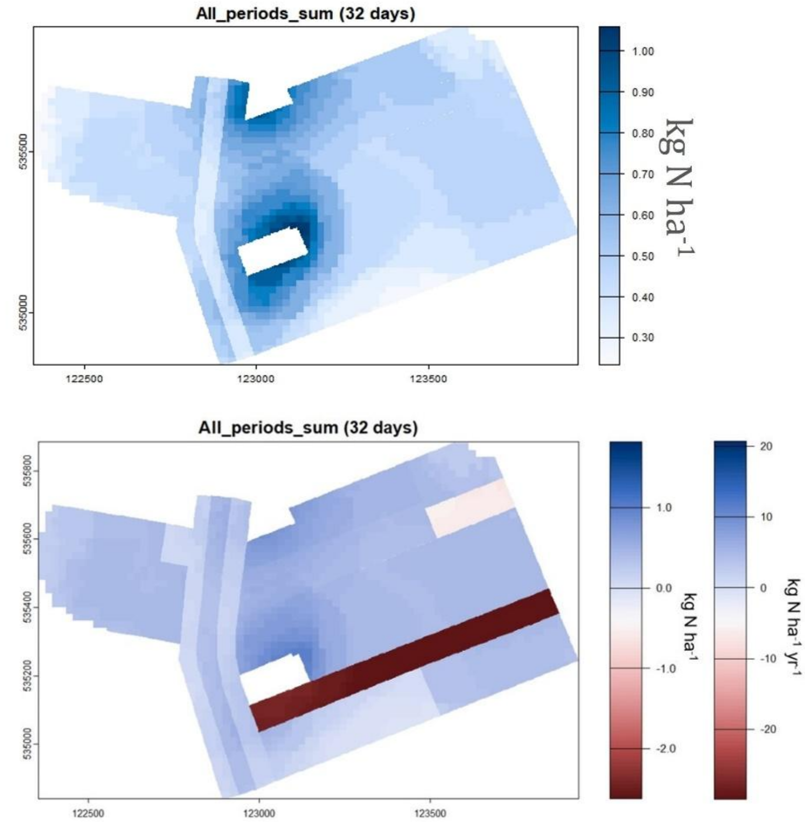


Figure 9 Spatially assessed NH_3 deposition near animal housing: Top panel: Surface independent deposition; Bottom panel: Surface dependent deposition.

2 Summary

The guidance on methods and uncertainty for determining spatial distribution of N deposition in the vicinity of animal housing for practitioners and regulators in this report provides practioners and scientists a range of options (Table 1, Table 3,Table 4) which summarise some of the currently available modelling and measurement approaches for assessing NH_3 concentrations in proximity of an animal housing and methods to progress from NH_3 concentrations to assessments of the NH_3 component of N deposition around a point source animal housing.

There are advantages and disadvantages of all approaches detailed here. The most essential part of planning NH_3 concentration and deposition measurements is having a clearly understood purpose and expectation of the effort which then allows the selection of the approach to be completed. The selection is also impacted by the resources available to deliver the measurements and modelling required.

Critical components of this are:

- Purpose and evidence requirements of the study
- Uncertainty requirements in monitoring
- Uncertainty requirements in modelling (if applicable)
- Method documentation
- Expert-developed and reviewed measurement plans
- Existing QAQC of methods
- What are the most important outputs of the monitoring?
    - Concentration field footprint
    - Deposition footprint
    - Concentrations across the landscape or at specific points
    - Model validation/calibration
- What will the monitoring outputs be used for?
    - N-deposition into proximate ecosystems to assess impacts against thresholds.
    - N-deposition into agricultural farmland to assess nutrient budgets, climate/NetZero studies.
    - Measurement of change and innovation across farm management system
    - Fraction of NH_3 emitted which “stays” on farmland.

2.2 Diffusive sampler network design

This Guidance designing a field monitoring study, before beginning N deposition assessments, many criteria and boundary conditions need to be considered:

- Complexity of emission landscape and if the source of interest can be sufficiently isolated Guidance from other emission sources in the landscape.

- Complexity of the geography and whether the model can take this into account.

- The agricultural cycle of the animal housing and ensuring the modelling and/or monitoring sufficiently captures the temporal change of the emissions over the cycle.

- The season of the modelling and/or monitoring and whether the monitoring sufficiently captures the temporal change of the emissions over the annual seasonal cycle.

- The local landscape background and variations through the agricultural calendar.

- The acceptable uncertainty at the edges of the footprint of the animal housing emissions (e.g. credible level and RMSE) which will allow modelling to be undertaken or verified.

- The acceptable uncertainty in proximity to the emissions in the footprint of the animal housing emissions (e.g. credible level and RMSE) which will allow modelling to be undertaken or verified.

Using the above criteria an approach can be designed. Great care needs to be taken if projecting beyond modelled area as it is not possible to make conclusions with statistical support about the distribution of NH_3 from the source outside of the modelled and/or monitored area, though suggestions with respect to trends continuing can be explored if clearly caveated.

Authorship:

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Appendices

Appendix A: Case Study 1: Bell et al. (2016) anaerobic digestion facility

Using the original dataset from Bell et al. (2016) the Bayesian model approach is applied to a network of 20 NH_3 samplers distributed around an anaerobic digestion facility for 6 periods. The method produces a spatial and temporally resolved estimate for NH_3 concentration around the anaerobic digestion (AD) facility, which is shown in Figure 11. The footprint of both the anaerobic digestion (AD) facility, and to a lesser extent a nearby dairy farm (which was on the periphery of the expected NH_3 footprint to the northwest), are present in all six of the study periods. The Bayesian model's "best fit" estimate also captures the effect of the prevailing wind on the concentration profile. A measure of uncertainty is given from the modelling iterations which can be used as an uncertainty estimate (Figure 12), giving what is called the credible range of the model output. This shows how much variation there is in confidence of the best fit estimate, i.e. the higher concentration that the model calculates as credible and the lower concentration across the model domain. A pattern is consistent over t periods 1-5, with a higher uncertainty (larger credible range) directly around the anaerobic digestion facility source (1 - 2.5 NH_3 µg m^3) and in the region to the west due to the dairy farm source. The final measurement period shows a much higher uncertainty range, possibly due to locally elevated NH_3 concentrations in this period.

The effects of distance from emission sources were isolated to see how these variables affected NH_3 concentration over space. These are mapped as a single time period to show the average effect of the emission source across the 6 time periods (Figure 14). The AD facility gives a highly concentrated point source of NH_3 with a steep concentration gradient, with some visible effect of the north easterly wind. The model predicts that the dairy farm gives a larger concentrated emission source with a larger emission profile compared to the AD facility (Figure 12). An example method for setting a threshold for the amount of acceptable uncertainty in the estimation of the NH_3 concentration field to demonstrate how the Bayesian modelling approach can be used to determine the spatial representativeness of a monitoring network. Figure 14 shows the credible range constrained to regions with a variability of less than 0.5 NH_3 µg m^3 (this threshold value was chosen arbitrarily for demonstration purposes). This removes the regions with higher variability, and when this spatial mask is applied to the best fit estimation (Figure 15), the areas to the north-west of the study area with more variable NH_3 estimates are not included in the representativeness area.

Due to the high density of sample locations around the AD facility, part of this region is included in the representativeness area for some time periods, despite much larger NH_3 values in these areas. Figure 16 shows the total representativeness area for the study site across the whole time period – quite a restricted region. This shows that the temporal variability in NH_3 concentration is substantial and affects the capacity of the monitoring network to accurately represent the concentration field at different points through the study period, reflecting different intensities of emission from the AD facility. The representativeness area here is restricted to an area that had low NH_3 concentrations recorded at the monitoring site across the study period. This process also shows the higher uncertainty levels, closer to the dairy farm, occur where there are fewer monitoring sites. In this specific example, due to access restrictions, the researchers were not able to place samplers within the fields surrounding the dairy farm which limited the capacity to detect the concentration gradient from the farm (this was discovered in the expert design discussion).

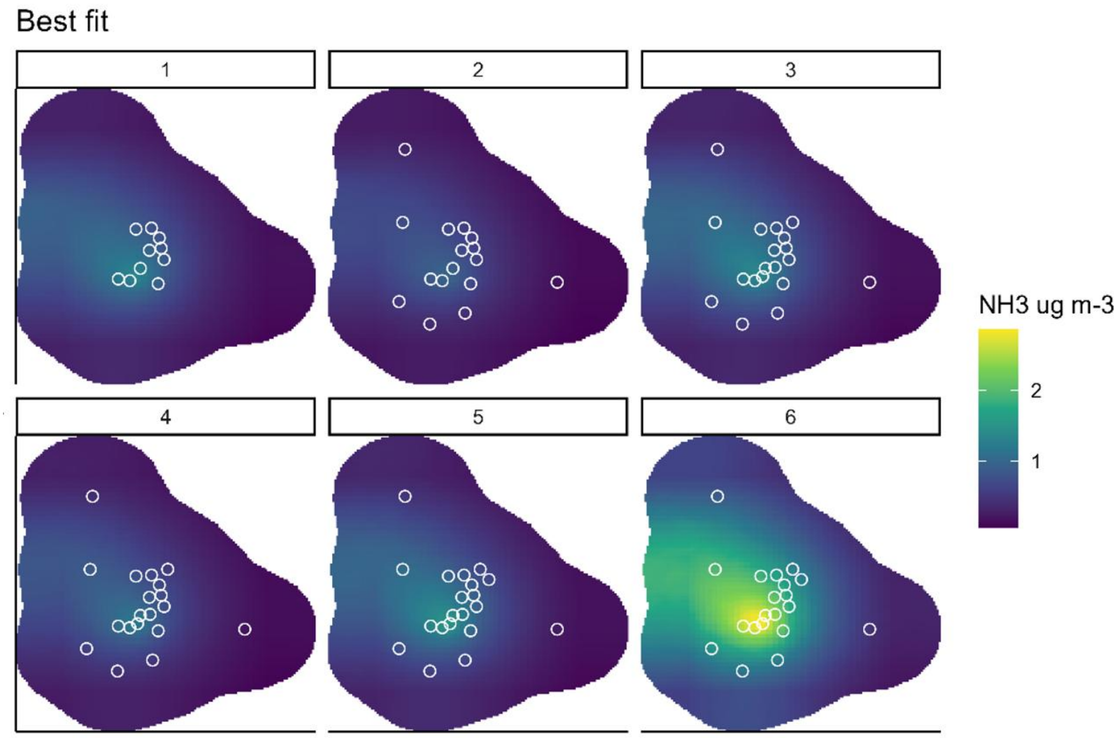

Figure 10 Spatiotemporal Bayesian model output for anaerobic digestion facility as an NH3 concentration field for each of the six measurement periods. Location of monitoring sites represented by white circles.

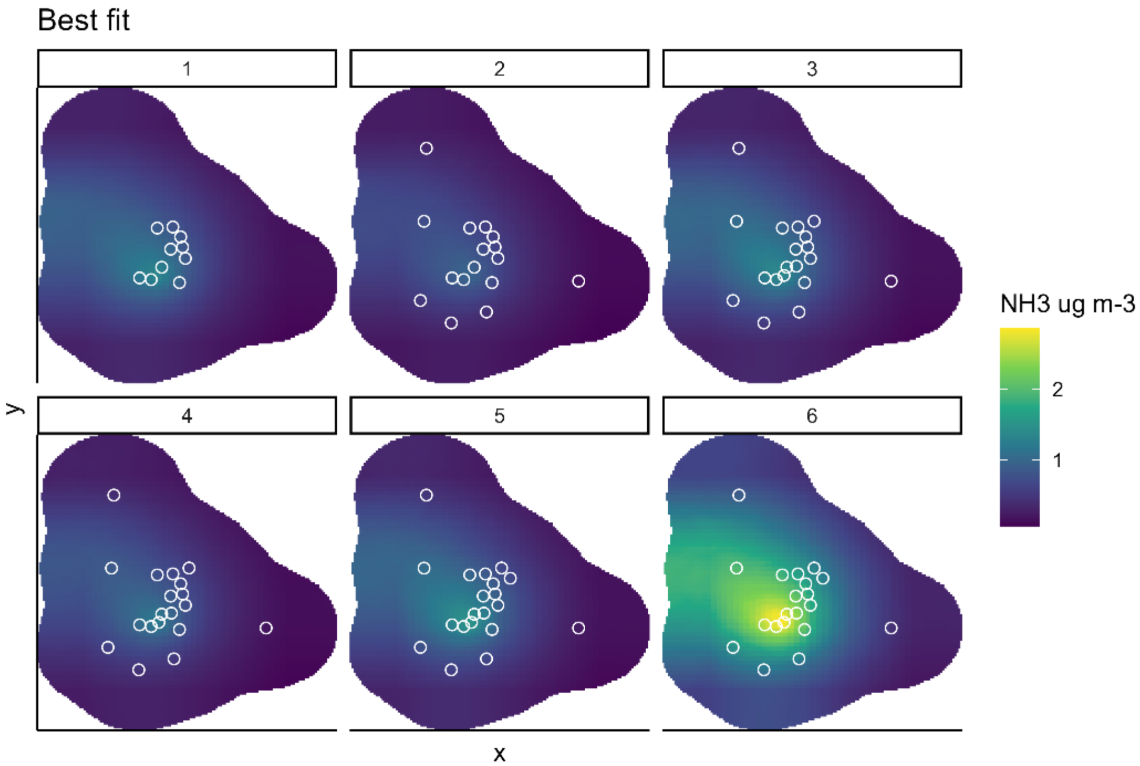

Figure 11 Spatiotemporal Bayesian model output for anaerobic digestion facility as an NH_3 concentration field for each of the six measurement periods. Location of monitoring sites represented by white circles.

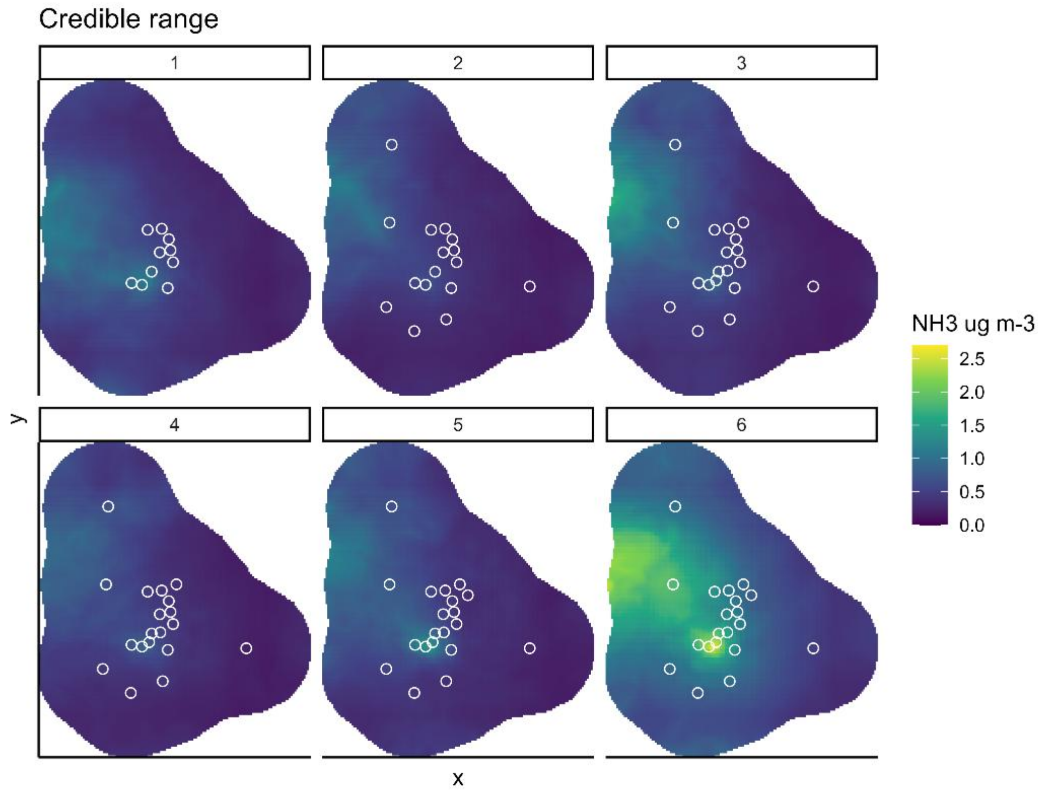

Figure 12 Estimate of range of uncertainty in the Bayesian model for each of the 6 periods of monitoring. The credible shows the difference in the high credible concentration and the lower credible modelled concentration. Location of monitoring sites represented by white circles.

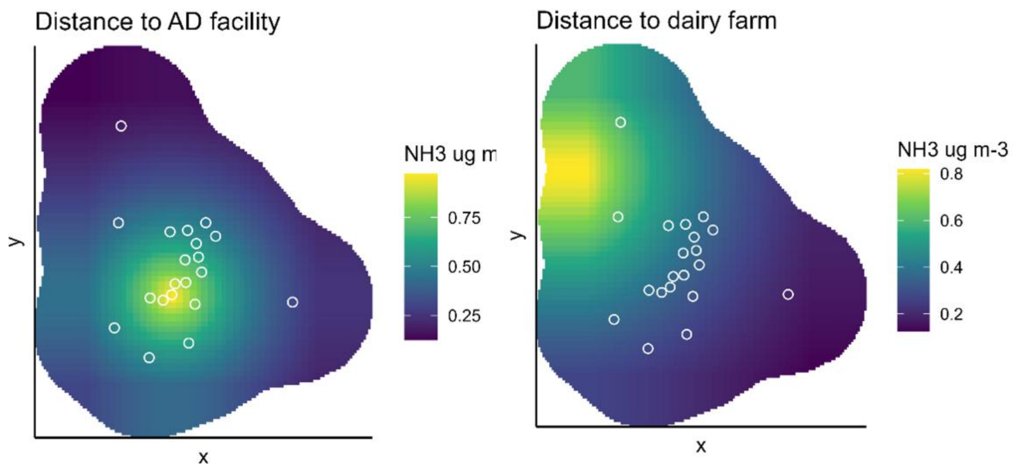

Figure 13 Isolated effects of distance from the anaerobic digestion facility (left) and dairy farm (centre) on NH_3 concentration field.

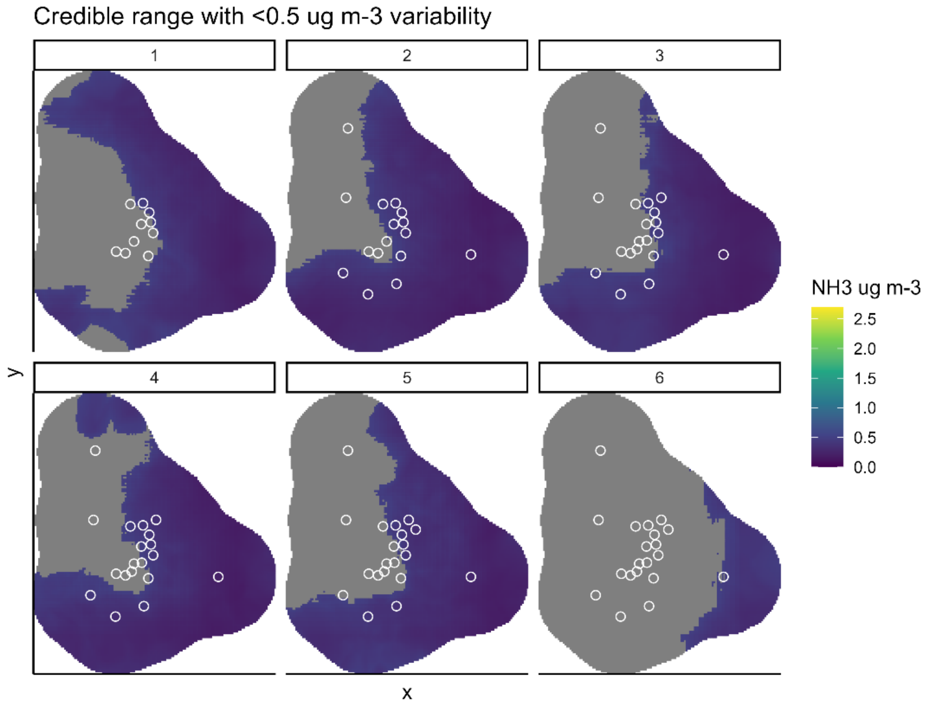

Figure 14 Credible range from Bayesian model with a 0.5 NH_3 µg m3 threshold applied – grey areas represent regions with variability higher than 0.5 NH_3 µg m^3 which are considered poorly represented in this example.

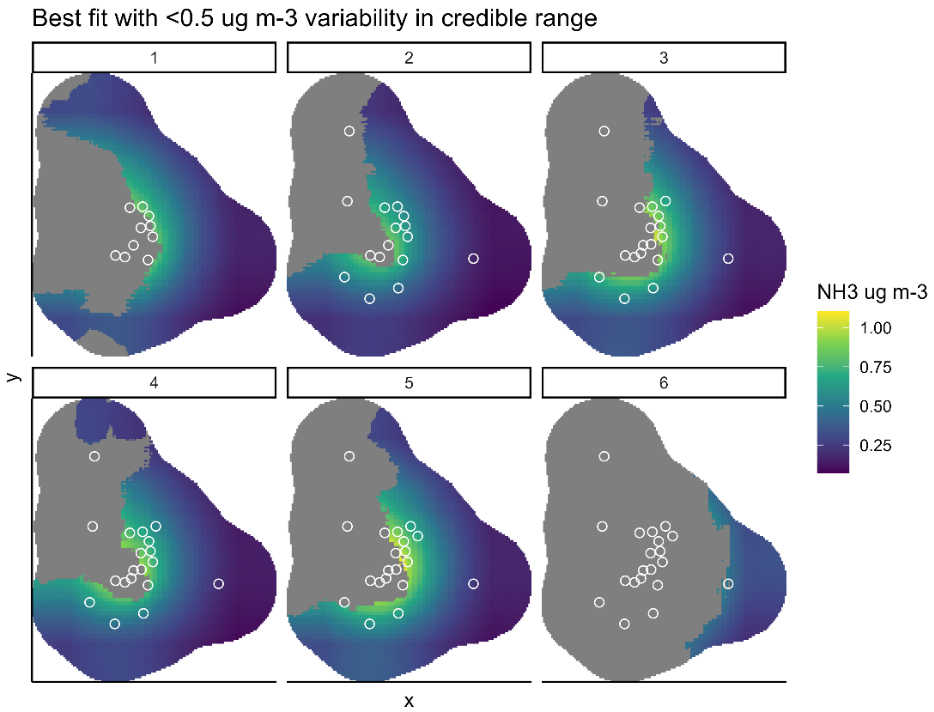

Figure 15 Representativeness of monitoring network when a 0.5 NH_3 µg m^{-3} maximum threshold of the credible range is applied the best fit of the Bayesian model.

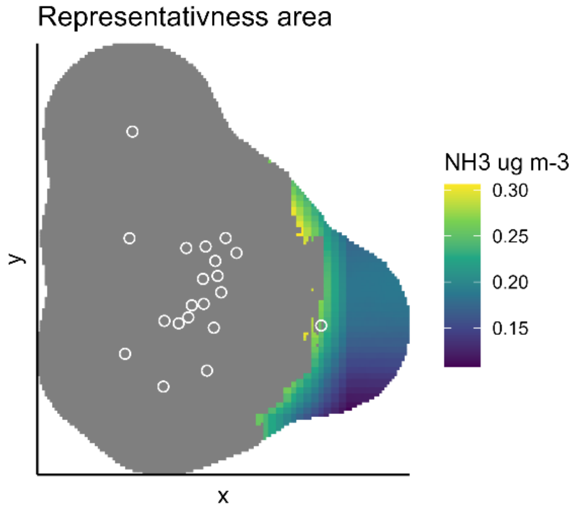

Figure 16 Overall spatial representativeness of monitoring network across the six time periods for capturing NH_3 concentration with <0.5 NH_3 µg m-[3] variability.

The Bayesian spatiotemporal modelling approach was undertaken for the same dataset but run with subsets of 19, 15, 10 or 5 monitoring sites (selected by 200 randomised reductions) and extracted the RMSE. It is important to note that there is a higher standard error of the simulations with 19 monitoring sites than the simulations with 15 or 10 sites included. This could be due to various reasons but not studied here. There are hundreds of thousands of possible combinations of sites that could be modelled with the 5, 10 and 15 site options. The distribution of RMSE values presented may not completely capture the full variability in the accuracy of the model fits. The distribution of NH_3 concentration is highly variable across space, so removing multiple monitoring sites from a simulation that are in close proximity to one another with a strong concentration gradient between them may actually result in an improved model fit. However, this does not mean that the model is giving a better representation of the concentration field, it is actually failing to capture even more of the variability in NH_3.

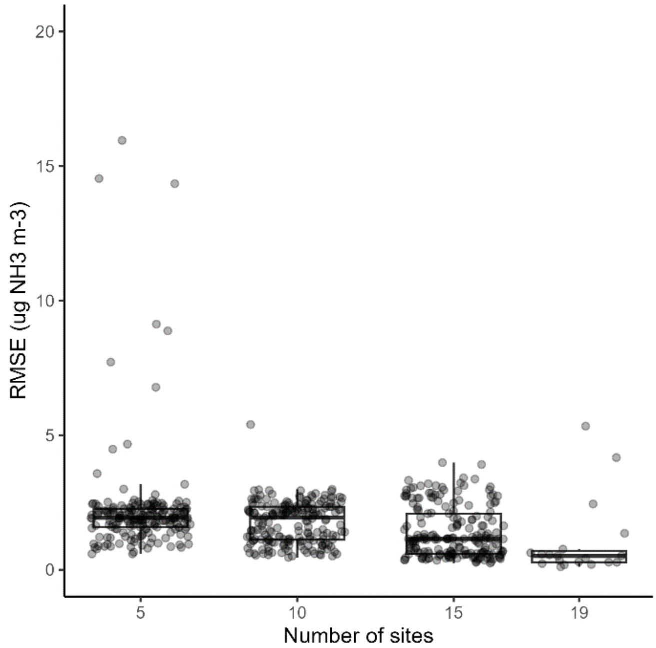

Figure 17 Root means square error (RMSE) values from subsetting the monitoring network to 5, 10, 15 or 19 sites from the original 20.

Table 7 Results from Bayesian model simulations with subsetted monitoring network sites (* there are only 19 possible combinations of models to run including 19 monitoring sites which is why there are fewer than the other sets of simulations)

Number of sites	Number of model runs	Mean RMSE from model runs (NH_3 µg m^3)	Standard deviation of RMSE from model runs (NH_3 µg m^3)
5	200	2.39	3.24
10	200	1.76	0.758
15	200	1.39	0.929
19	19*	1.01	1.44

Appendix B Case Study 2: Hill et al. (2014) poultry farm

The Bayesian spatiotemporal model fitted to data from the 9 ALPHA samplers over the four time periods from Hill et al. 2014 best fit and credible range are presented in **Error! Reference source not found.**. In comparison to the AD facility from Bell at al. 2016, the concentrations reported here are substantially higher, peaking at 50 NH_3 µg m^3 directly around the farm in the first three monitoring periods. It is important to note that the spatial scale in this example is larger than the AD farm example (Bell et al. 2016), with the modelled area here representing 0.5km^2. The final period, after the chicken sheds were cleared, has negligible NH_3 concentrations. As there is only one emissions source in this example, the best fit represents the extent of the emissions profile from the single poultry farm.

The modelling to simulate monitoring networks with fewer samplers shows a clear trend of reduced error in estimated NH_3 concentrations as the number of monitoring sites increases (**Error! Reference source not found.**). 4 and 6 monitoring sites show high RMSE values that also vary substantially amongst simulations, whereas the simulations using 8 monitoring sites have a much lower RMSE (Table 8). This example shows a clearer trend of the effect of reduced RMSE with lower numbers of monitoring sites on model quality than the AD example, which could be attributable to the more complex emissions sources at the AD study site.

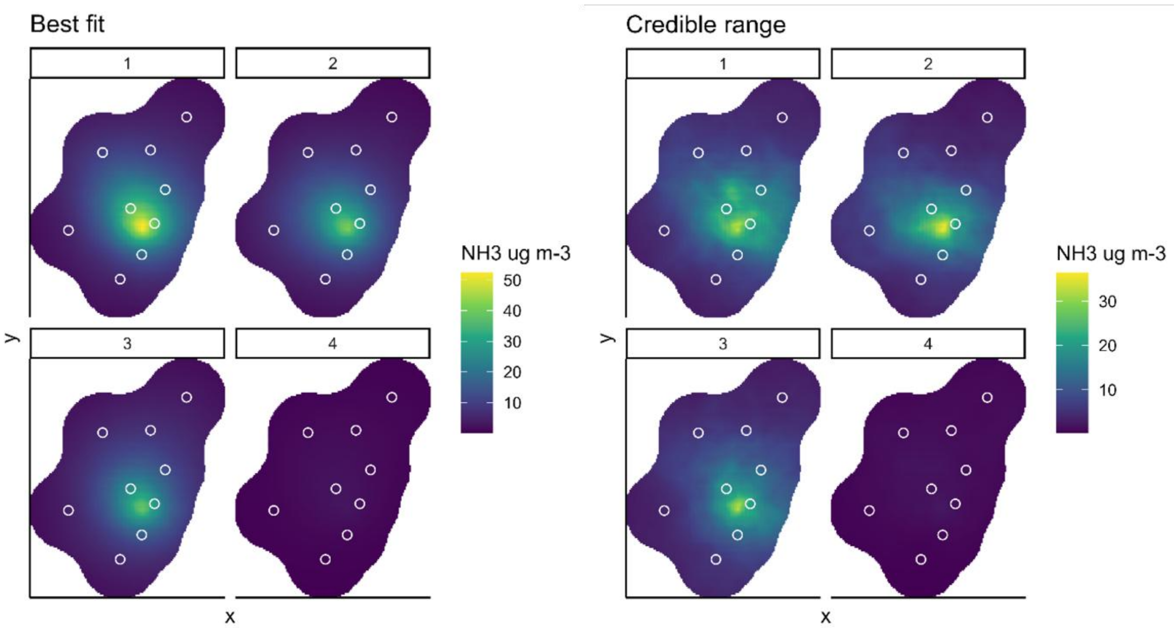

Figure 18 Best fit (left) and credible range (right) for Bayesian spatiotemporal model fit for NH_3 concentration around poultry farm. White circles indicate sampler locations.

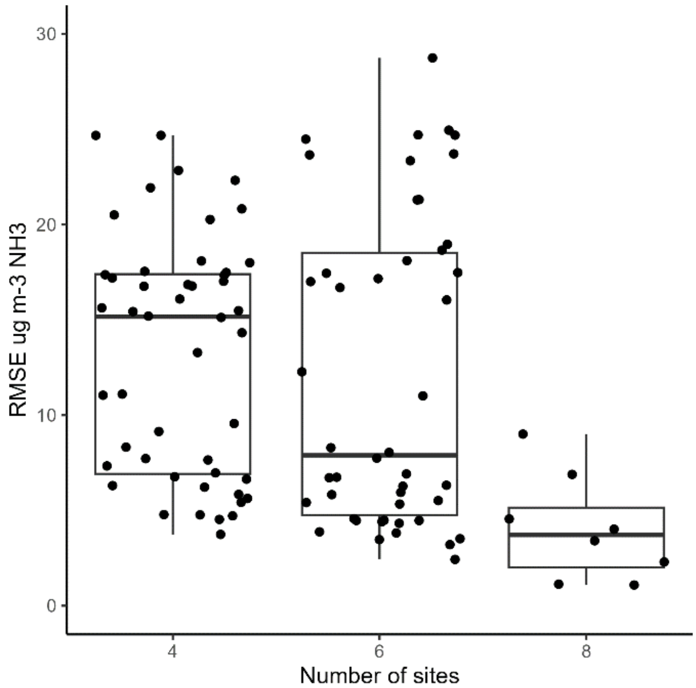

Figure 19 RMSE values for simulations of subsets of monitoring sites from the monitoring network.

Table 8 Results from Bayesian model simulations with subsetted monitoring network sites (*there are only 8 possible combinations of models to run including 8 monitoring sites, which is why there are fewer than the other sets of simulations)

Number of sites	Number of model runs	Mean RMSE from model runs (NH_3 µg m^3)	Standard deviation of RMSE from model runs (NH_3 µg m^3)
4	50	13.2	6.23
6	50	12.0	8.12
8	8	2.77	2.77

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