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Higher tier estimation of ammonia emissions from synthetic nitrogen fertilizers in emission inventories: data collation, methodology and analysis

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ABSTRACT

Synthetic fertilizers are a key source of ammonia (NH_3) emissions globally and national emission inventories are an essential element of international agreements aimed at reducing these emissions. Here an analysis of published measurements of NH_3 emission from synthetic fertilizer found that emissions were primarily determined by the experimental approach, the chemical composition of the fertilizer, environmental variables and the method of application. Measurements made using wind tunnels, semi-open chambers and the micrometeorological method produced similar results whereas those made with closed or ventilated chambers, Dräger tubes or ^{15}N were lower. Measurements made outdoors were lower than those made in the laboratory. The most important factors determining the NH_3 emissions were the method of application, the chemical composition of the fertilizer and, for fertilizers not based on solid forms of urea, the soil pH. National inventory compilers normally take account of these factors but are encouraged to use more detailed methodologies. Here we present a range of statistical models that would allow inventory compilers to also take into account application rate, air temperature, rainfall and soil clay content. However, to take advantage of these models would require the availability of additional, good quality input data.

The conditional R^2 of the models developed accounted for 44–55 % of the variance in NH_3 emission measurements but the marginal R^2 only 19–27 %. We recommend further investigation into the source of the low marginal R^2 and, in particular, into the differences caused by the use of the different measurement methods.

1. Introduction

Ammonia (NH_3) emissions contribute to the formation of fine secondary particulate matter ($PM_{2.5}$) in the atmosphere (Behera and Sharma, 2010; Schiferl et al., 2014), which is considered to have negative effects on human health (Xing et al., 2016; Nieder and Benbi, 2022). Deposition of NH_3 or its reaction products leads to eutrophication of nitrogen (N) sensitive ecosystems (Dise et al., 2011) and to the emission of nitrous oxide (N_2O), which is a greenhouse gas (IPCC et al., 2006). As a consequence, European emissions of NH_3 are regulated by the Gothenburg Protocol of the UN Convention on Long-Range Transboundary Air Pollution (CLRTAP) (UNECE, 2005) and the EU National Emissions Ceilings Directive (NECD) (EU and Union, 2016), and must be reported under the UN Framework Convention on Climate Change (UN, 1994).

The EMEP/EEA Air Pollutant Emission Inventory Guidebook ('the Guidebook') (European Environment Agency, 2023a) is the official reference document for compiling emission inventories in connection with the CLRTAP and NECD while the IPCC Guidelines (IPCC et al., 2019) is the official reference document for reporting under UNFCCC. The IPCC Guidelines have global scope while the geographic scope of the Guidebook is in principle Europe and North America.

The relative importance of different emission sources varies between countries and this determines whether IPCC and UNECE allow the use of a simple Tier 1 methodology or require the use of the more detailed Tier 2 methodology. The Tier 2 methodology represents a compromise

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between the desire to take account of the factors determining an emission and the anticipated ability of emission inventory compilers to obtain the activity data associated with those factors. Consequently, where the data permit, inventory compilers are encouraged to improve the accuracy of their emission inventories by using a Tier 3 methodology. Tier 3 methodologies include any that are more detailed than Tier 2, so can range from methods using an enhanced emission factor (EF) approach through to those based on complex process-oriented modelling. Properly used, Tier 3 methodologies provide emission estimates that are more accurate than Tier 1 and 2. As importantly, their greater detail is useful when determining priorities for the implementation of abatement measures and assessing their likely applicability.

In the context of emission inventories, a methodology consists of a model and guidance on how to parameterize and use that model. A number of models to predict NH_3 emission from synthetic N fertilizers are already available, varying with respect to their objective and function. These range from dynamic models that describe the underlying mechanisms in some detail (Sherlock and Goh, 1985; Rachhpal-Singh and Nye, 1986; Génermont and Cellier, 1997; Garcia et al., 2011; Dutta et al., 2016; Michalczyk et al., 2016), through less detailed process-based models e.g. (Ismail et al., 1991; Misselbrook et al., 2004; Nyord et al., 2008; Fillery and Khimashia, 2016; Pacholski et al., 2017) to those using EFs (Bouwman et al., 2002; Macnack et al., 2013; Ma et al., 2021b). The statistical work by Pan et al. (2016) quantifies the effectiveness of measures to reduce NH_3 emissions, relative to those occurring from broadcast urea, rather than the effect of the conditions driving those emissions. Process-based models that include all the major factors that influence NH_3 emissions have the potential to generate a more accurate inventory and create a better basis for assessing the likely impact of reduction measures. However, a large number of factors are known to affect the emissions (see below), meaning that process-based models of NH_3 emissions demand large numbers of parameters and input data. Using such models for wide-area (inventory) purposes would require substantial resources for data acquisition or collation, to avoid this demand introducing model bias and uncertainty. Examples of the use of models of varying complexity for estimating wide-area NH_3 emissions can be found in the literature e.g. (Xu et al., 2019; Zhan et al., 2021; Beaudor et al., 2023), but none are currently in use for official reporting under UN conventions. One of the barriers to the use of such models is that while their documentation is adequate for the purpose for which they were developed, it is not adequate for use in national emission inventories.

From discussions within the UNECE Task Force on Emissions, Inventories and Projection (TFEIP), it is apparent that the additional technical expertise and resources for data acquisition needed to use complex, process-based models for emission inventories represent a significant barrier for their use in a number of countries. There is therefore a need to develop simpler, statistical models that allow countries to move beyond the current Tier 2 methodologies of the Guidebook and Guidelines, at a tempo consistent with the resources at their disposal. The purpose of this study was therefore to develop and document a range of Tier 3 models of NH_3 emissions from pure-form synthetic nitrogen fertilizers.

2. Methods

2.1. Data sources

Reports of empirical studies of NH_3 emissions were identified as follows:

- From the database of literature compiled by Bouwman et al. (2002) (accessible from http://www.pbl.nl/en/publications/2002/Estimation_of_global_NH %3Csub %3E3 %3C/sub %3E_volatilization_loss_from_synthetic_fertilizers_and_animal_manure)
- From the survey of scientific literature undertaken in 2012 by the Department of Environmental Sciences, Aarhus University, for the European Environment Agency, as part of a re-assessment of the Tier 1 and 2 methodologies for NH_3 emission in the Guidebook (these methodologies were published in the 2016 version).
- From the database collated by Pan et al. (2016) and kindly made available to the authors.
- Through contacting colleagues in the field (especially with regards to reports not published in reviewed journals)
- By searching the bibliographic database Web of Knowledge for the years 1970 to present*.
- By Google searches*.
- From references in publications found by the above means.

* using the following keywords: ammonia and emission or volatili* and fertili*.

Data were omitted if a. the chemical composition of the fertilizer could not be identified, b. if emissions were expressed in relative terms only (e.g. relative to urea), c. if the experimental design was incomplete or could not be understood, d. if it was clear that the duration of the experiment was insufficient to capture the whole of the emission event and e. if the emissions were for periods with prolonged sub-zero temperatures. The latter restriction was applied because of a fear that the short-term nature of most experiments would fail to capture the full emissions. Engel et al. (2017) found emissions from urea applied to continuously frozen soil to continue for more than 3 months. Finally, for a number of reasons, experiments on paddy rice were also excluded. The first is that the cultivation practices in paddy rice differ greatly from those of dryland cropping, so their inclusion could distort the analysis for the latter systems. The second is that we are aware of a significant body of data that is not accessible to us, as it has been reported in non-English language journals and reports (principally in Chinese). Thirdly, the area dedicated to rice production in North America and in Europe only represents 0.7 % and 0.3 % respectively of the global total (FAO, 2025). Finally, rice production systems in Europe and North America deviate significantly from those in Asia (Hill et al., 1991).

Since in all experiments, the background NH_3 concentration or capture was subtracted from measurements obtained from fertilized treatments, some negative emission values were reported in experiments investigating low-emission fertilizers. With one exception (see below), these data were retained in the dataset to avoid truncating the variation in emission measurements.

The processes driving NH_3 emissions from synthetic N fertilizers are well known and generally well understood (Harrison and Webb, 2001; Sommer et al., 2004), although there remains a lack of knowledge on process interactions. Since NH_3 emissions from synthetic N fertilizers are predominantly driven by physical and chemical processes, data was collated from scientific reports, with a global scope. The main focus was on peer-reviewed publications but non-reviewed reports were included, where the quality of the work appeared adequate to our criteria.

2.2. Choice of environmental variables for collation

The main mechanisms driving NH_3 emissions from synthetic fertilizers (Fig. 1) have been known for many years (see e.g. Harrison and Webb (2001)) and many have been included in models designed for wide-area application (e.g. Bouwman et al., 2002; Ma et al., 2021a; Zhan et al., 2021; Rathbone and Ullah, 2024).

Ammonia is only emitted from the soil when ammonium (NH_4^+) is present in solution. Ammonium is formed either when fertilizers containing NH_3 or ammonium salts are dissolved in water or when urea is hydrolysed. The NH_3 volatilisation rate increases with increasing temperature, wind speed and pH, while the presence of an anion in the fertilizer decreases emission, to an extent that depends on the type of anion. Some of the NH_4^+ in soil solution is reversibly bound to negatively-charged ions and humus compounds in the soil (cation

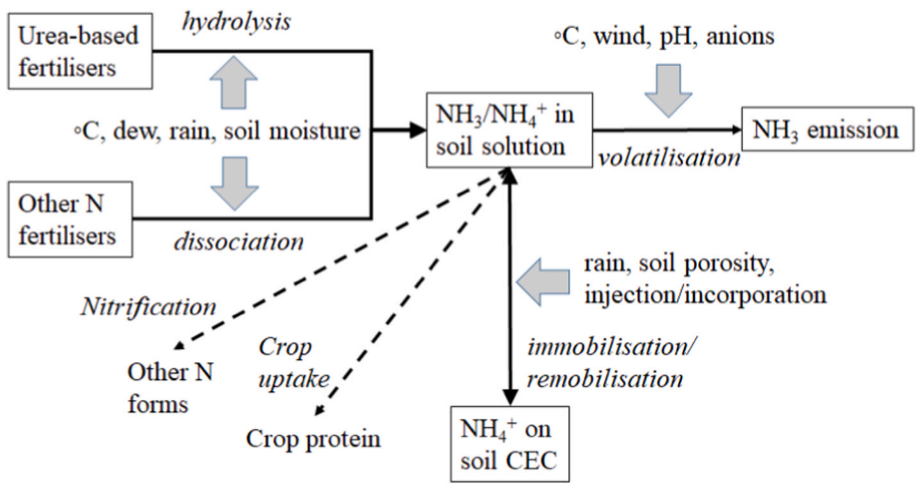


Fig. 1. Mechanisms determining NH_3 emission from synthetic fertilizers.

exchange capacity, CEC), reducing emission. Any process or management activity that transports the NH_4^+ down into the soil reduces volatilisation, partly by increasing the exposure to the CEC and partly by increasing the resistance to NH_3 transport to the atmosphere. The processes and activities include injection or incorporation of the fertilizer and rain- and irrigation-driven vertical transport. Ammonium is nitrified by soil organisms and taken up by the crop, both of which reduce the NH_4^+ available for volatilisation. However, these processes generally occur at a slower rate than soil adsorption and volatilisation.

The processes shown in Fig. 1 can be classified into three main groups; 1. those relating to the properties of the fertilizer and its application, 2. those relating to the soil to which it is applied and 3. those relating to the conditions at the time of application and thereafter. For group 1, the chemical composition of the fertilizer was noted, as was the application rate (kg N ha^{-1}). To avoid excluding too many data, applications made using injection and rapid incorporation were included, using the following categories: solid broadcast; liquid, injected or incorporated. For incorporation, no distinction was made between ploughing and other methods such as harrowing, or the depth of either. For group 2, the soil properties recorded were pH (without distinction between measurement method), and soil CEC (without distinction between measurement method, CEC; $cmol_c$ kg^{-1}). However, we found that CEC was reported with only moderate frequency. The soil CEC is determined primarily by the clay and organic matter contents, so we recorded the clay content (%) and soil organic carbon contents (g kg^{-1}). Where the soil texture was reported but clay content was not, the soil texture triangle (USDA et al., 2017) was used to obtain an estimate of the latter. For group 3, we recorded the crop type (including bare soil). The initial soil moisture status and wind speed were rarely reported and were not included here. Mean air temperature (Celsius) and cumulative rainfall (mm) for the 7 days after application were recorded where possible, as were mean air temperature and cumulative rainfall for the duration of the experiment. Since irrigation is a common crop management practice, studies that included irrigation after fertilization were included and irrigation amount included as an explanatory variable. Some temperature and rainfall data were transcribed from graphs, meaning that the accuracy with which both variables were noted varied among publications. A summary of the data collated is given in Table 1 below:

Table 1
Summary of data recorded.

Data	Units	Data	Units	Data	Units
General information					
Authors	–	Year	Year of publication	Country	Location of experiment
Location	Laboratory or outdoor	Measurement method	[a]	Duration of experiment	Days
Number of replicates	–				
Cumulative loss of NH_3– N	%	Standard deviation			
Fertilizer and application					
Chemical composition	[b]	Application method	[c]	Application rate	kg N ha^{-1}
Soil					
Soil type	[d]	Clay	%	Soil pH	–
Soil CEC	$cmol_c$ kg^{-1}	Soil organic carbon	g kg^{-1}	Crop cover	[e]
Conditions					
Air temperature - first 7 days	°C	Air temperature - mean for duration	°C	Rainfall - first 72 h[f]	Mm
Rainfall - cumulative for duration[f]	mm	Irrigation - cumulative for duration[f]	mm	Wind speed - mean for first 7 days	m s^{-1}

[a] Micrometeorological, Ventilated chamber, Closed chamber, Wind tunnel, ^{15}N, Drager-Tube, Semi-open chamber.
[b] Urea (U), Ammonium nitrate (AN), Ammonium sulphate (AS), Urea ammonium nitrate (UAN), Monoammonium phosphate (MAP), Diammonium phosphate (DAP), Calcium ammonium nitrate (CAN), Ammonium bicarbonate (ABC), Urea phosphate (UP), Double urea phosphate (UUP), Urea ammonium sulphate (UAS).
[c] Broadcast, Incorporated, Sprayed, Injected.
[d] Clay, Sandy clay, Sandy clay loam, Sandy loam, Sand, Loamy sand, Loam, Clay loam, Silty clay, Silty clay loam, Silt loam, Silt.
[e] None, Cereal, Grass, Maize, Trees, Rape, Cotton, other.
[f] After fertilizer application.

2.3. Choice of methodological data collated

Emission data were recorded as the NH_3-N emitted, expressed as a proportion of the fertilizer N applied, cumulated for the whole measurement period reported. Most data were reported as the mean of two or more replicates, so only mean values were collated. Since, the standard deviation was infrequently reported, the replicate number associated with each observation was also recorded. If the number of replicates was not reported in a publication, it was assumed that there was no replication.

Experiments conducted outdoors are more likely to represent the conditions occurring in agricultural practice than those in the laboratory, but it can be difficult to avoid confounding effects outdoors. For laboratory experiments, the situation is reversed. Furthermore, a range of methods is used to obtain estimates of NH_3 emissions (see for example Herrero et al., 2021). The methodological data collated consisted of whether the observations were from outdoor or laboratory experiments, the measurement method and the duration of the measurement period. A wide range of methods are used for the measurement of NH_3 emissions (Scotto di Perta et al., 2020). For the purpose of the present analysis, the measurement methods were classified into micrometeorological (i.e. all free air methods, irrespective of detector technology), wind tunnel, ^{15}N and four types of chamber methods; closed chamber (no air exchange), semi-open (open at the top), ventilated (pumped air exchange) and Dräger-Tube (Pacholski et al., 2006).

3. Statistical analysis

The literature sources from which data were collated are in Supplementary Information S1. The data were analysed in two groups; all data and only data from outdoor experiments. Full details of the statistical analyses will be made available on GitHub, where the repository will be made public upon acceptance.

3.1. Categorisation of data

There were few observations of NH_3 emission following application of a number of fertilizers (Table 2). To increase the ability to quantify the effect of different fertilizers despite small sample sizes for individual fertilizers, the data were stratified into larger categories. The aim here was to create categories that a statistically meaningful number of observations, while retaining as much chemical specificity as possible. This resulted in 4 categories, according to the similarity of the chemical composition of the fertilizer; 1. Urea++ consists primarily of urea, with a small number of other solid, urea-based fertilizers, 2. UAN differs from the other urea-based fertilizers since it is applied as a liquid, so its interaction with the soil might be expected to differ and there was a sufficient number of observations to support the statistical analysis, 3. Ammoniun+1 is a group of solid fertilizers with all of the N in the form of ammonium and 4. Ammonium+2 consists of two solid fertilizers, where half the N is supplied as ammonium and half as nitrate. Only 14 reports of NH_3 emissions after application of anhydrous ammonia were found in the literature, 6 of which were more than 50 years old. Anhydrous ammonia is applied by injection as a liquid but rapidly converts to a gas after application. Given the age and paucity of the data and that its rapid conversion to a gas meant it could not be readily placed into one of the four groups, we chose not to include anhydrous ammonia in the model development.

Likewise, the cropping data was aggregated into 4 groups; none, arable, grass and other. The location of outdoor experiments was categorised into one of three agro-ecological zones (temperate, sub-tropical and tropical).

We used NH_3-loss, expressed as % of N applied, as a response variable. The NH_3-loss was calculated as the difference between the NH_3 emissions from a fertilized treatment and those from an unfertilized control. On examination, the assumptions of residual normality were not met for the data. Having investigated a range of transformations (logarithmic, square root, cube root), a square root transformation was found to be the most effective method to normalize the residuals. Negative emission observations were present in a number of studies and in one study (Velthof et al., 1990), some were substantially negative. We interpreted the substantial negative values in Velthof et al. (1990) to be experimental artefacts and the whole study was omitted from the analysis. We consider the remaining negative values to reflect statistical variation in the method used measure the emission from the fertilizer and control treatments. Thus although physically meaningless, these data contain valuable statistical information and would result in biased estimates of emissions, were they to be omitted. To accommodate the remaining marginally negative values in the square root transformation, we therefore applied a constant of +4 % to all observations. This constant was subtracted, when transforming effect sizes into emission factors. The bias introduced by the addition of the constant was explored with a sensitivity analysis and found to be minor (Supplementary Information S2).

In developing inventory methodologies, there is much emphasis on transparency and, thus, on the use of methods for which the benefits and pitfalls are well known. Consequently, for the statistical analysis, we chose to take a frequentist approach, rather than using machine learning methods. Given the unbalanced nature of the collated dataset, the number of observations available for analysis decreases as the number of variables included in regression equations increase. The strategy adopted was therefore to first fit a base model containing key explanatory variables. Additional explanatory variables were then screened to determine whether there was a basis for combining them with the base model, to create one or more additional models with additional variables. The results of experiments for which the base model variables were not available were not included in the dataset used for analysis. The screening processes consisted of first parameterizing the base model using the whole dataset, thus providing the best estimate of the effect of the base variables. For each of the additional variables, a subset of the data was then created that only contained the results of experiments in which the additional variable was reported. In this subset, we fitted a linear model containing only the additional variable as a fixed predictor variable and the NH_3 loss as a response variable. We added the fitted values of the base model as an offset variable. The offset variable is accounted for in the model estimation by subtracting the fitted values from the observed emissions, thus ensuring that the analysis is done on the residual variation, but the results are reported in the units of the original response. If the analysis of this new variable found a significant effect ($\alpha = 0.05$), the additional variable was subject to further analysis. This further analysis consisted of regressing the NH_3-loss against the base variables and one or more of the additional variables, to create a range of models. To assess the contribution of each variable in the base model, we conducted a variance component analysis by repeating the linear mixed effects model with all variables set as random effects.

The variables chosen for inclusion in the base model were fertilizer

Table 2
Fertilizers and fertilizer categories.

Compound	Abbr.[a]	N[b]	Fertilizer category
Ammonium bicarbonate	ABC	10	Ammonium+1
Ammonium sulphate	AS	230	Ammonium+1
Diammonium phosphate	DAP	44	Ammonium+1
Monoammonium phosphate	MAP	23	Ammonium+1
Ammonium nitrate	AN	286	Ammonium+2
Calcium ammonium nitrate	CAN	80	Ammonium+2
Urea ammonium nitrate	UAN	116	UAN
Urea ammonium sulphate	UAS	18	Urea+
Urea phosphate	UP	27	Urea+
Double urea phosphate	UUP	11	Urea+
Urea	Urea	1393	Urea+

[a] Abbreviation.
[b] Number of observations.

category, application method, measurement method and, for the full dataset, location. These variables were chosen because both theory and previous studies indicated that they have a major impact on NH_3 emissions; The additional explanatory variables were chosen using the criteria that they 1. should be recorded for all or the great majority of the observations, 2. from scientific theory and/or previous experimentation have a major effect on emissions, and 3. be potentially obtainable by inventory compilers. The additional variables were application rate, soil pH, soil clay content, soil organic carbon content, soil cover, mean air temperature for the experimental duration, mean 7 day air temperature, mean daily rainfall for the experimental duration (mm day^{-1}), cumulative irrigation after fertilization, water input rate i.e. mean total rainfall + irrigation (mm day^{-1}) and experimental duration (days).

The data suggested that the relationships between NH_3 and rainfall intensity (mm d^{-1}), and between NH_3 and the soil clay content were non-linear, so an exponential function of the following form was fitted for the outdoor datasets:

$$y = ae^{bx} \tag{1}$$

where y = non-linear rainfall or non-linear clay, x = rainfall intensity (mm d^{-1}) or soil clay content (%), and both a and b are constants.

The non-linear rainfall and non-linear clay were included as an explanatory variable.

In general, we could not examine interactions among explanatory variables, since this would exclude all observations from experiments in which one or more of the variables was not measured. This would have reduced the dataset for analysis substantially. With two exceptions, we therefore made the assumption that there is no significant interaction between the variables examined. The two exceptions are fertilizer category and soil pH, and air temperature and rainfall. In the first case, earlier work has found a significant interaction (Ohnemus et al., 2021). In the second case, an initial analysis of the data from outdoor studies found a significant positive correlation using Pearson's method ($r = 0.30$, $p < 0.001$, based on 932 observations).

To account for heteroscedasticity, we used weighted ordinary least squares (WOLS, Olvera Astivia and Zumbo, 2019). We built a vector giving larger weight to observations with smaller variation. To this end, we extracted absolute residuals and fitted values from an unweighted version of Model 1. We then applied a regression model between the absolute residuals (response variable and fitted values (predictor variable)), to estimate the relationship between the amount of variation and the data and the model estimates. To attain a vector with higher values attached to lower variation, we used the inverse of the relationship estimated in the regression model. The weights correspond to increased weight with decrease in variation, thus giving more precedence to more accurate data. The R^2-values for linear mixed effects model were calculated according to Nagakawa and Schielzeth (2013).

4. Results

4.1. Data collated

A total of 2604 cumulative NH_3 emission measurements were collated from 257 publications (see S1 Supplementary Information for the full list of references). The number of observations (mean values in case of replicated treatment measurements) per publication ranged from 1 to 111, with a mean of 10 and a median of 5.

The dataset is available without restriction from https://doi.org/10.3220/253-2025-14-

The distribution of measurements between fertilizer categories is shown in Table 3.

About 40 % of the observations were from experiments in which the emission was measured using ventilated chambers, with closed chambers accounting for a further 30 % (Table 4). The other methods accounted for 10 % or less of the observations. Ventilated and closed chambers were used in both outdoor and laboratory locations, with the other methods used mainly or exclusively outdoors. Most fertilizer was applied by broadcasting, as either a solid (68 %) or liquid (18 %), with few observations for injection or incorporation. Application to bare soil was most common (58 %), followed by arable (28 %) and grassland (13 %). There were 1411 observations from outdoor experiments and 1185 from laboratory experiments.

Table 3
Grouping of fertilizer types and their representation in the database and usage statistics.

Fertilizer category	N	% of obs[a]	% by use: Europe	% by use: World
Urea++	1729	67	20	49
UAN	128	5	13	6
Ammonium+1	365	14	20	30
Ammonium+2	374	14	42	9
Other[b]			3	6

[a] Percentage of observations.
[b] Including anhydrous ammonia.

The global distribution of observations is shown in Fig. 2. The continental distribution of observations was Europe (798), N America (909), Asia (377), Oceania (158), S America (227) and Africa (127).

4.2. Models developed

Full details of the statistical analysis, including the R code, are available at DOI: 10.5281/zenodo.18174795. For the observations from both outdoors and in the laboratory, there were significant effects of fertilizer category, measurement method and application technique in both base models (all data or just outdoor) and of the location (laboratory or outdoor). The variance component analysis of all data showed that fertiliser type, application method, measurement method, and location explained 17 %, 5 %, 4 % and 9 % of the total variance, respectively. 42 % of variation was unexplained by the model, and 24 % was attributed to the literature reference.

The screening process suggested that the variance accounted for by the base model would be significantly increased by including one or more of the additional explanatory variables shown in Table 5. The significant terms varied, depending on whether all data or only outdoor data were used.

Although there was a significant relationship between the NH_3 emission and the non-linear clay function, the departure from linearity was considered insufficient to justify the additional complexity.

For the whole dataset and for the outdoor data, there was no significant relationship between the residuals from the base model and soil CEC (1612) or soil organic carbon (1486). For the outdoor data only, there was no significant relationship between the residuals from the base model and the following variables; agro-ecological zone (1408), irrigation (1101), mean water input per day (rainfall + irrigation) (1043), mean daily rainfall during the experiment (1037), 7 day rainfall (673), and air temperature and rainfall, with the inclusion of the interactive term (933). For the raw data (as opposed to the residuals from the base model fit), there was a significant ($p < 0.05$) non-linear relationship between NH_3 and mean rainfall (933). For the residuals from the base model, the relationship with the non-linear rainfall variable (as opposed to mean rainfall) and air temperature was significant ($p < 0.05$) (933) but not if the interactive term was included. Further analysis showed that the relationship with mean air temperature and mean rainfall, including the interactive term, was significant ($p < 0.05$) if the mean air temperature was between 1 °C and 22.6 °C (Fig. 3). The relationship indicates that the negative effect of rainfall on NH_3 emissions increases, as the air temperature decreases.

The variables found to be significant in the supplementary models were included in a series of additional multivariable models (Table 6). In addition to the base model variables, soil pH and the interaction between soil pH and fertilizer category were significant in all cases. Air

Table 4
Variable summaries, divided by fertiliser types. Sample sizes (n) are presented for categorical variables, and median and range (minimum and maximum observation) for continuous variables.

Names		Urea+	UAN	Ammonium+1	Ammonium+2
Total (n)		1729	128	365	374
Place	Outdoor (n)	964	108	141	198
	Lab (n)	765	20	224	176
Application method	Broadcast (n)	1184	3	262	325
	Incorporated (n)	275	9	58	8
	Injected (n)	5	116	45	41
	Liquid (n)	265	0	0	0
	Micrometeorological (n)	149	31	20	5
	15N (n)	5	43	147	119
	Closed chamber (n)	465	4	10	3
	Drager-Tube (n)	148	24	21	26
	Semi-open (n)	97	26	160	156
	Ventilated chambers (n)	692	0	7	65
	Windtunnel (n)	173	0	0	0
Application rate		100 [15,927][a]	133 [38,200]	100 [15,400]	100 [15,400]
Soil pH		6.5 [3.6,9.4]	6.4 [4.6,9.3]	7.4 [3.6,9.3]	6.5 [4.1,9.1]
pH	normal - ≤7 (n)	1047	78	151	233
	chalky - >7(n)	991	991	991	991
Clay (%)		17 [0,89]	18 [5,70]	15 [0,72.1]	15 [0,72.1]
Soil organic carbon (%)		9.7 [0.1310]	19 [2,36]	0.9 [0.2125]	7.4 [0.1125]
Soil organic carbon	mineral (n)	578	12	115	162
	organic (n)	441	55	51	74
Cover	arable (n)	511	69	54	96
	grass (n)	204	8	35	85
	none (n)	999	51	274	192
	other (n)	15	0	2	1
Rainfall (mm)		22.6 [0,383]	23 [0,255]	44.5 [0,325]	26.1 [0,383]
Air temperature (°C)		20 [-5,45]	19 [0,34]	20.2 [4.3,38]	20 [-1.3,32]
Irrigated (n)	No (n)	578	88	72	162
	Yes (n)	196	6	293	212
Water (mm/day)		1.5 [0,25]	1.3 [0,6.4]	1.3 [0,10.6]	1.5 [0,19.1]

[a] [minimum value, maximum value].

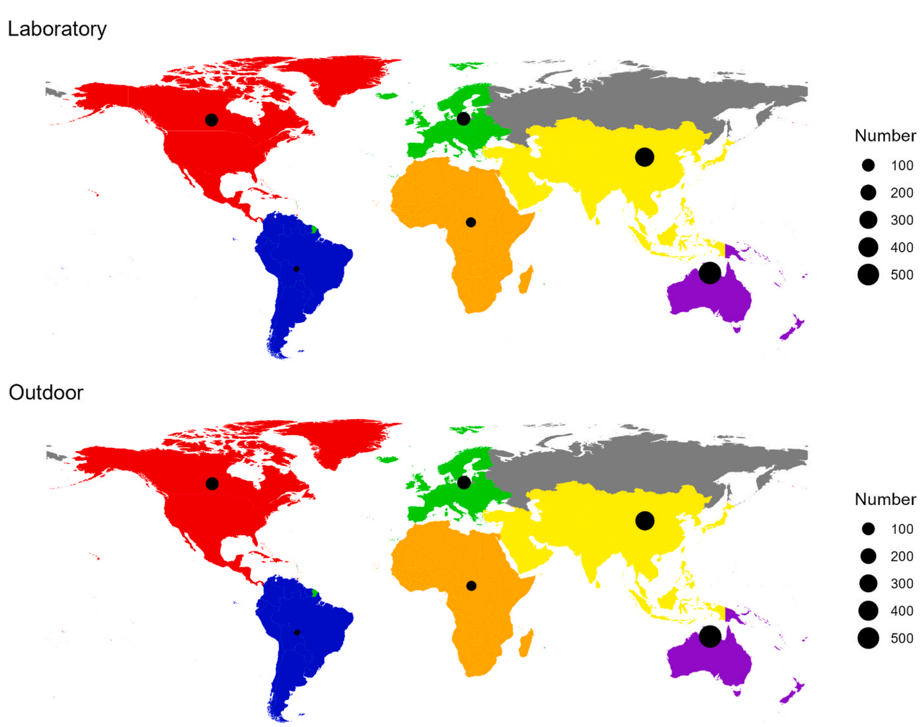


Fig. 2. Geographic distribution of measurement data (top = laboratory, bottom = outdoor).

temperature was not significant in all models but was significant for models based both on data from all locations and just from outdoors. In contrast, the application rate was only significant in three models based on outdoor data, while the clay content was only significant in two models based on all data. The model including application rate, mean air temperature, mean rainfall and the interaction between mean air temperature and mean rainfall was retained, even though the latter interaction was not statistically significant for the whole range of air

Table 5
Significance of the effect of explanatory variables in the subsidiary models (all and outdoor data).

Variable	All data	N	Outdoor only	N
Soil pH	***	2501	NS	1356
Soil pH x Fertilizer category	***		***	
Application rate	NS[a]	2076	*	1367
Clay content	*	2356	NS	1236
Air temperature	**	1897	*	1054

a. NS = not significant ($p > 0.05$), *$p < 0.05$, **$p < 0.01$, ***$p < 0.001$.

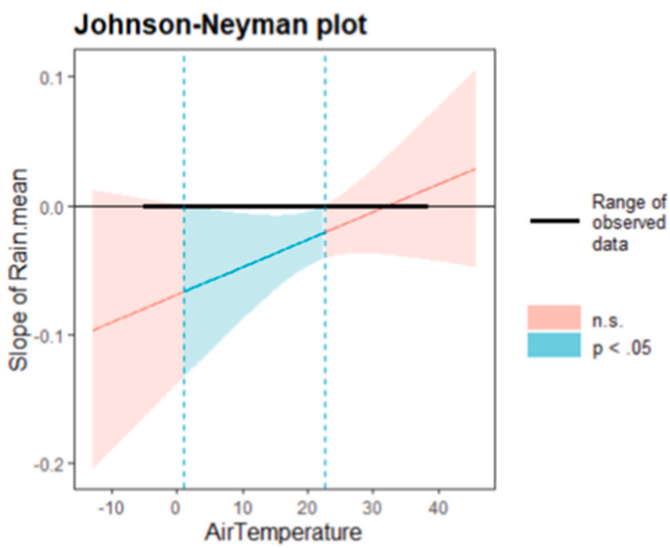


Fig. 3. Zone of significance for the relationship between the residuals of the base model and mean air and mean rainfall.

temperatures. This was because the interaction is significant over a range of air temperatures that are relevant in temperate regions of the world.

The most complex model including all data (Model A4) was cross-validated with leave-one-out cross-validation. We find a RMSE value of 1.41, which equates to 10 % of the raw average. Correlation between predicted values and true values in the cross-validation resulted in a sample correlation coefficient of $r = 0.55$.

The coefficients of these models are in Supplementary Information S3, together with guidance on how to use the parameters in the models. Worked examples of the models in Excel format are in Supplementary Information S4.

The fixed effects of categorised variables for Model A1 and Model LO1 are shown in Fig. 4.

The effects are smaller for the outdoor data but otherwise display a similar pattern to those when data from both laboratory and outdoor locations are included. The emission from incorporated and injected fertilizer is less than from surface-applied fertilizer (Liquid or Broadcast). The fertilizer category with the highest emission is Urea+, which consists mainly of pure urea. The emission from UAN is about half that of the Urea+. The emission from the Ammonium+1 is lower still but higher than from the Ammonium+2. The emission from the fertilizers that contain ammonium (Ammonium+1, Ammonium+2 and UAN) is higher when they are applied to chalky soils (pH > 7) than to normal soils, whereas there is little effect of soil pH on the emission from the fertilizers that only contain N in the urea form. The soil pH *per se* had little effect. The measurement methods fall into two groups with regards to emissions, with wind tunnels, semi-open chambers and micrometeorological methods measuring similar values, but higher than those measured using ventilated chambers, closed chambers and ^{15}N methods.

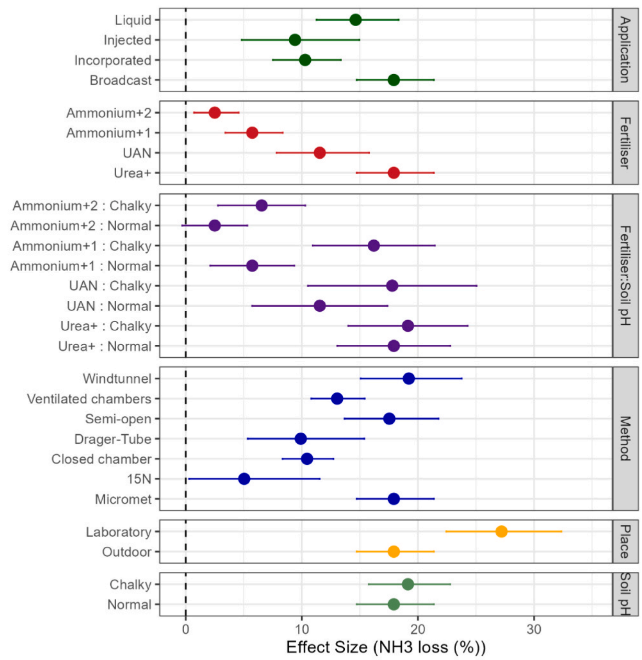
5. Discussion

5.1. Partitioning of the variance

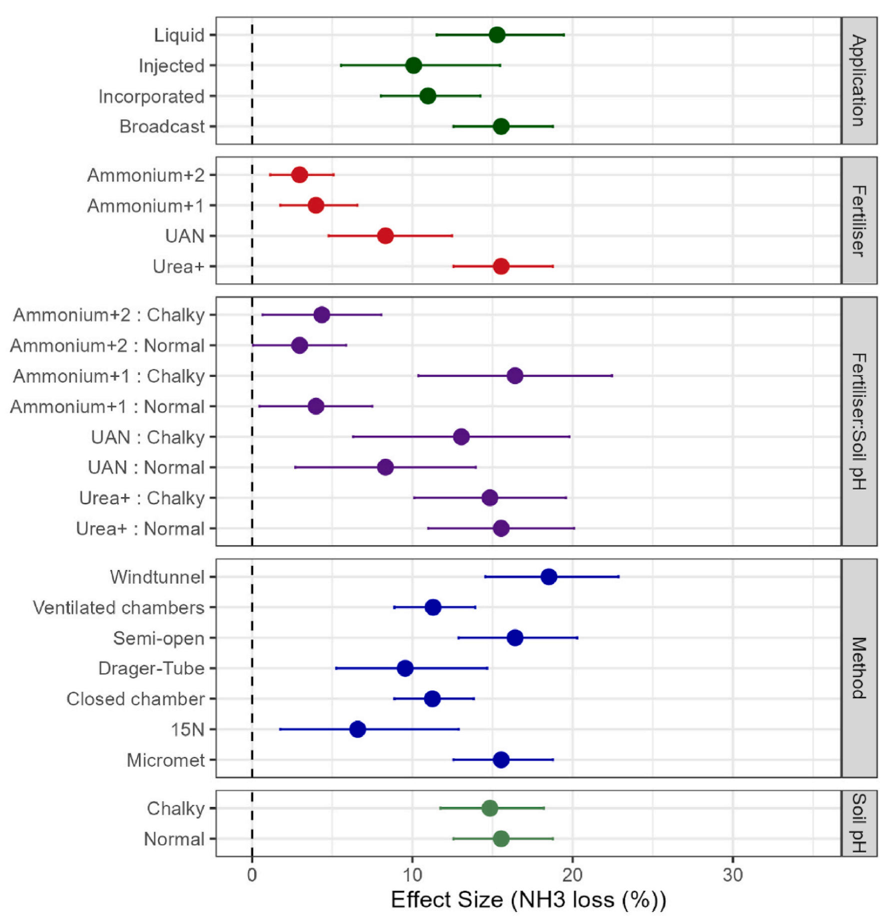
The statistical analysis partitions the variance between three components; that which can be attributed to the explanatory variables, that which can be attributed to the source of the data (i.e. form which study the data were taken) and that which cannot be specifically attributed. The partitioning varies between models but the three components account for roughly 25 %, 25 % and 50 % of the variance respectively. As noted earlier, the NH_3 emission from N fertilisers is determined by a complex range of interacting factors, so it is inevitable that the relatively simple models developed here cannot explain a large proportion of the variance in the data. It is concerning that a relatively large proportion of the variance is associated with the source of the data. This is despite our attempt to characterise the individual studies in terms of the location (laboratory or outdoor) and measurement methodology. In part, this may be due to differences between studies in the relationship between the choice of explanatory variables (e.g. air temperature, rainfall) and the conditions at the site of emission (e.g. soil surface temperature, soil moisture). This is unavoidable, in part because the latter data were not normally available from the data published and in part because these data would not normally be available to emission inventory compilers. The explanatory variables are discussed in detail below.

Table 6
Levels of significance and numbers of observations for additional models.

Variable	All data				Outdoor only				
	Model								
	A1	A2	A3	A4	LO1	LO2	LO3	LO4	LO5
Fertilizer category	***	***	***	***	***	***	***	***	***
Application technique	***	***	***	***	***	***	***	***	***
Measurement method	***	***	***	***	**	***	***	***	**
Indoor/outdoor	***	***	***	***	NR	NR	NR	NR	NR
Application rate						***		***	***
Soil pH	***	***	***	***	***	***	***	***	***
Soil pH x Fertilizer category	***	***	***	***	***	***	***	***	***
Clay content		***		***					
Mean air temperature			***	***			***	***	*
Mean rainfall									*
Rainfall x air temperature									NS
Number of obs.	2500	2295	1855	1693	1355	1317	1034	1025	923
Marginal R^2 (%)	23.5	25.2	24.6	27.0	18.2	19.0	19.9	20.9	18.5
Conditional R^2 (%)	50.3	53.5	51.4	54.8	43.8	45.7	45.0	47.6	45.5
AICc	7610	6919	5611	5079	7647	6084	5626	5612	2612
RMSE	1.04	1.01	1.02	1.00	1.045	1.02	1.03	1.02	0.90



a. All data



b. Outdoor data only

Fig. 4. The model estimates for the fixed effects of a. Model A1 and b. Model LO1. Lines indicate the 95 % confidence limits. For a given target explanatory variable, the estimates were obtained by parametrising the non-targeted variables to Application = Broadcast, Fertilizer type = Urea+, soil pH = normal, Measurement method = Micromet, and Location = Outdoor.

5.2. Explanatory variables – measurement methodology

The absence of a significant relationship between NH_3 emissions and the duration of experiments indicates that the data collated captured most or all of the emission events.

As found by Bouwman et al. (2002), the estimated NH_3 emission was significantly higher for experiments conducted indoors compared to outdoors. This difference remained when both measurement method and air temperature were included in the model (Model A3). In the laboratory studies, the soil structure present in the field is not retained and rain effects are not generally considered. Similarly, the relationship between the air temperature and the temperature at the site of NH_3 volatilisation is likely to have been differences between the two locations, e.g. due to differences in the long and shortwave radiation environments. However, the measurement methods are broadly defined categories, with variations in their implementation (Scotto di Perta et al., 2020). Only two measurement methods were used extensively both the laboratory and outdoors (closed and ventilated chambers – see Table 4) and it is possible that there were significant differences in their implementation between the two locations. Such variations exist even for the micrometeorological method, which is considered the one most likely to reflect *in situ* emissions; a recent comparison of measurements made with this method in a single experiment found substantial differences within different implementations (Kamp et al., 2024). These variations in implementation may explain why the explanatory power of the models was relatively low (19–27 %), with the random effects, which reflect the study from which the data were obtained, generally accounting for a similar proportion of the variance as the fixed effects.

The similarity between the micrometeorology, semi-open and wind tunnel methods is encouraging, since the micrometeorology method requires substantially more resources than the latter, thus severely limiting both treatment and replicate numbers. However, the substantial within-method variation remains a concern. There needs to be a concerted effort to reduce the variation between research groups in the emissions measured using the same method. This requires a collaborative effort between groups, similar to that which resulted in the special section in Journal of Environmental Quality *GRA N2O Chamber Methodology Guidelines* (JEQ, 2020). A detailed overview of measurement methods will be included in the forthcoming revision of the UNECE Ammonia Guidance Document (Bittman et al., 2014). However, there is a strong case for more experiments in which the different measurement methods are compared with one another and with known emissions from a reference source. When conducting experiments to investigate a range of ammonia emission abatement measures, it is impractical and/or expensive to use the large plot size necessary when using the micrometeorological measurement method. It is therefore important to assess the validity of small-plot methods in determining the relative reduction in emissions.

5.3. Explanatory variables – chemical, management and environmental factors

As anticipated from physical and chemical principles, and the earlier work of Bouwman et al. (2002), the NH_3 emissions were significantly related to the chemical composition of the fertilizer, soil pH and application technique. The Urea + fertilizer category has the highest NH_3 EF but displays the lowest effect of soil pH. The hydrolysis of urea leads to an increase in the pH of the soil solution, which promotes NH_3 emission (Rachhpal-Singh and Nye, 1986). The extent of the pH increase depends on the buffering capacity of the soil. Where urea-based fertilizers are applied as solid, the effect of the urea hydrolysis on soil pH is concentrated in the soil immediately adjacent to the granules. This means that the local pH is raised substantially and NH_3 emission is higher than for other fertilizer categories. Furthermore, the localised nature of the effect reduces the buffering effect of the soil, so the difference between the emissions on calcareous and non-calcareous soils is smaller than for other fertilizer categories. The lack of the effect of hydrolysis in fertilizers where the N is only in the ammonium form (ammonium+1) means that the pH environment adjacent to the granules is largely determined by the soil, so the NH_3 emission from calcareous soils is elevated compared to that of non-calcareous soils. For the ammonium+2 fertilizer category, half the N is in the form of nitrate, so has no or only a negligible effect on NH_3 emission. Since the EF is expressed as the mass of NH_3-N per unit mass of N applied, the EF is about half that of the ammonium+1 category. With UAN (30 % N grade), the contributions to the total N are 41 % urea, 39 % ammonium and 20 % nitrate, so about 80 % of the N is either directly or after hydrolysis in an ammonium form. Furthermore, it is applied as a liquid, in form of big droplets or liquid bands, not a solid, so compared to Urea+, the localised effect of urea hydrolysis on pH should be much smaller and the soil pH should have a stronger effect on NH_3 emission. The EF for UAN is indeed intermediate between Ammonium+1 and Urea+ and lower at the normal soils than on the calcareous soils.

There were significant effects on emissions of the soil clay content (only for all data), air temperature and rainfall (only for outdoor data), although inclusion of these variables only marginally increases model accuracy. A decrease in emission with increasing clay content would be expected from physical and chemical principles (see above), although the reduction found here is less than has been found in practice (Pelster et al., 2019). The absence of a significant relationship when only using outdoor data was due to the smaller number of observations and the absence of soils that contained little or no clay.

A positive relationship between emissions and air temperature would also be expected from physical and chemical principles (see above and in Lei et al., 2017) and was found in practice by Zhan et al. (2021) for emissions from synthetic fertilizer and manure. When considering the suitability of using models that include air temperature as an explanatory variable for inventory calculations, it is necessary to assess the extent to which the correlation between air temperature and rainfall in the data might affect the parameterisation. An examination of the slope of the relationship between NH_3 emissions and air temperature for models developed using outdoor data was similar to that developed using laboratory data only (where the rainfall effect is absent), suggesting that the rainfall effect on the relationship with air temperature is minimal.

Our understanding of the processes driving NH_3 emission would suggest that there would be a negative relationship with rainfall, possibly a non-linear dilution effect. While there is such a relationship if it is tested as a single factor, when included with air temperature in a complex model, it is only significant when combined with a marginally non-significant interactive term. Both these environmental variables are included as means over the duration of the experiment, since there were no significant relationships when considering the period immediately after application (probably due to a very limited dataset). It is possible that the longer and the shorter term temperature data are more closely related than for the rainfall i.e. the rainfall data are more representative of climate than weather. In this connection, it is worth noting that (Ma et al., 2021a) found a significant positive relationship between NH_3 emission and mean annual precipitation.

The relationships with temperature and rainfall raise the possibility of achieving abatement by timing fertilizer applications to coincide with conditions that would not favour NH_3 emissions. A quantification of the effectiveness of such optimal timing is beyond the scope of this paper, since it would be dependent on the degree of variation in meteorological conditions (i.e. the potential for exploitation) and any factors that constrain the ability of farmers to exploit that potential in practice (e.g. crop nutritional requirements).

5.4. Explanatory variables – management factors

The lower emission when fertilizer is injected or incorporated results from the increased interaction of NH_4^+ with the soil cations and the increased resistance to NH_3 transport to the free atmosphere. The current investigation did not find a significant effect of irrigation, even though an understanding of the processes and a number of empirical studies (e.g. Holcomb et al., 2011; Viero et al., 2017) have shown it to significantly reduce NH_3 emissions. In the current investigation, irrigation was mainly registered as part of routine crop management and not specifically as an NH_3 abatement measure i.e. timed to occur immediately after fertilizer application.

The models developed here can be used to assess the effect of replacing high-emission fertilizer types with lower-emission types. However, we do not recommend the use of the models developed here to quantify the effect of other abatement measures such as incorporation, injection and irrigation. The categories used lack detail (e.g. distinguishing between shallow and deep injection, or irrigation amount) and there are relatively few data. Quantifying the effect of abatement measures requires more detailed study and a comparative approach, based on relative rather than absolute emission reductions. In this respect, more research is necessary to understand the extent to which smaller scale, lower cost measurement methods can replace or supplement the micrometeorological method, which is considered to give the most reliable quantitative estimate of NH_3 emission under *in situ* conditions.

5.5. Comparison with previous studies

A number of studies using the results of a meta-analysis of NH_3 emission data have been published over the last three decades, with recent publications focussing on estimates of global NH_3 emissions or to investigate measures to reduce NH_3 emissions from synthetic fertilizers. Where these are the objectives, it is not always feasible to determine the EFs used or, where process-oriented models are used, calculate implied EFs from the results (e.g. Xu et al., 2019; Beaudor et al., 2023). In other cases (e.g, Aneja et al., 2020), separate EFs were not identified for the four fertilizer categories used in the current study. Table 7 shows the EFs found by a number of previous studies, with the models are parameterized for broadcast application, micrometeorological method and outdoor (field) experiments where appropriate.

While the different studies agree that the largest EFs are for urea-based fertilizers and the lowest for Ammonium+2, there are important differences, especially in the effect of a high soil pH on emissions from the different fertilizer categories. The reason(s) for these differences are unclear. Fewer measurements were available to Asman (1992) and Bouwman et al. (2002). Bouwman et al. (2002) and Ma et al. (2021a) both included measurements of NH_3 emission from manure application in their models, as well as synthetic N and both included additional land uses (e.g. paddy rice). Note that NARSES differs from the other studies as it combines potential EFs for each fertilizer category with a simple representation of the driving processes.

5.6. Use of models in national emission inventories

Official national emission inventories differ from those created at national or international scales for scientific purposes, as they are produced as part of international agreements or legislation and thus have legal status. They are required to follow good inventory practice (European Environment Agency, 2023a) and are subject to periodic independent review.

The models developed here are based on data from global sources but the geographic distribution is uneven (e.g. few data available from Africa in particular, Fig. 2). However, NH_3 emission from synthetic fertilizers is driven primarily by fundamental chemical and physical processes (Fig. 1), though for urea, also by the indirect effect of the biological processes that generate the urease enzyme. We therefore consider the models to be globally applicable, if the explanatory variables are within the range of values used in the development of each model.

The models developed only accounted for a relatively small proportion of the variance in the observations. We concluded above that the large proportion of the variance that cannot be attributed to a specific source in the current analysis was due to the number of factors determining NH_3 emissions from N fertilisers and the complexity of their interactions. Increasing the accuracy of estimates of NH_3 emissions from this source requires using models that can account for more factors and interactions than those developed here. However, as noted in the Introduction, the use of such models demands a significant investment of resources for the collection, collation and use of activity data. Furthermore, additional resources are required when using such models in emission inventories, to maintain good inventory practice in relation to documentation and transparency. Although parameter estimates in the models developed are associated with significant uncertainty (so any individual observation has a high uncertainty), the RMSE value of the most complex model represents 10 % of the raw average, so the average effects have a high predictive accuracy.

Inventory compilers are obliged to use a Tier 2 methodology (if it is available) for the most important (key) sources of emission but are encouraged to migrate to a Tier 3 methodology, if it would increase the accuracy of the inventory. For NH_3 emissions from synthetic fertilizers, the Tier 2 methodology in the 2023 Emission Inventory Guidebook (European Environment Agency, 2023b) is based on Model A1, parameterized for broadcast/liquid application, outdoor studies and the micrometeorological measurement method (though with coefficients from an earlier version of the analysis and fewer data). The decision concerning the number of factors to include in the Tier 2 methodology for a compound depends particularly on whether we think most countries can be expected to obtain the associated activity with sufficient accuracy. The EFs in the 2023 Emission Inventory Guidebook are therefore dependent on the fertilizer type and the soil pH but not on other factors known to affect emissions (Fig. 1). As the analyses undertaken here and in other studies have shown, other factors can significantly affect the EFs, so if there are substantial differences in these other factors between a given country or region and the data used for the development of the Guidebook Tier 2 EFs, using the Tier 2 methodology could result in considerable bias. In this case, moving to a Tier 3 methodology, based on one of the models developed here, has the potential to reduce the bias of the emission estimates and provide a better basis for decisions concerning abatement strategies. Inventory compilers

Table 7
NH_3 emission factors from this and earlier studies.

Fertilizer category	Normal pH			High pH			All pH	
	Bouwman et al. (2002)	NARSES[a]	Model LO1	Bouwman et al. (2002)	NARSES[a]	Model LO1	Asman (1992) [b]	Ma et al. (2021)
NH_3-N emitted (% of N applied)								
Urea+	12.7	15.9	15.5	17.6	15.9	14.8	15	14.3
UAN	3.1	8.1	8.3	4.3	8.1	13.1	8	7.3
Ammonium+1	8.0	1.8	4.0	11.0	15.9	16.4	4–8	4.1
Ammonium+2	3.4	1.8	3.0	4.7	1.8	4.4	2	2.9

[a] Version from 2015.
[b] Also used by (Goebes et al., 2003).

would however need to be aware that such a move will only be successful in this aim if the additional activity data required can be obtained with an acceptable quality. The resulting emission estimates might still have a relatively high uncertainty but will be less uncertain than if the Tier 2 methodology were used.

As an alternative approach to the use of the models developed here, some inventory compilers may be in a position to develop their own models, based on data from a more geographically restricted area. This is only possible if a substantial body of emission data is available or can be collected via empirical experiments, for climate, soil and management conditions relevant for the geographic scope of the inventory. If feasible, this approach is to be preferred, since the EFs will be more thoroughly founded in the local agricultural conditions.

Inventory compilers considering a migration to a Tier 3 methodology that incorporates one of the models developed here are advised to consider the following factors:

1. Is the model valid for the range of the variable(s) in the target country? At a minimum, this means within the range defined by the minimum and maximum value(s) of the variable(s) in the dataset used to develop the model.
2. Would the inclusion of additional variables significantly impact the emission estimates, either now or in the future? For example, is the range of air temperature or application rate in the target country sufficient to result in a significant change in the EF?
3. Is it technically, legally and financially possible to obtain the necessary input data with a quality that does not bias the estimate?

The latter point will often be the greatest barrier to moving to a Tier 3 methodology, since the explanatory variables must be available with a high spatial and/or temporal resolution. How the bias relative to the Tier 2 methodology changes with the spatial and temporal resolution of input data will vary between the model in question and be dependent on the variation in the explanatory variables at the target geographic location. The temporal resolution is a particular issue for models that include air temperature and rainfall, even though they are based on mean values for the duration of experiments (the mean duration was 20 days). High temporal and spatial soil and interpolated meteorological data are available for some regions (e.g. for Europe, from https://esdac.jrc.ec.europa.eu/resource-type/european-soil-database-soil-properties and https://agri4cast.jrc.ec.europa.eu/DataPortal/Index.Aspx respectively) but utilizing these data requires at minimum a knowledge of the date and location of applications of the different fertilizer categories.

When using one of the models presented here to estimate EFs, to obtain values that most accurately reflect conditions in practice, we recommend that they are parameterized for broadcast/liquid application, outdoor studies and the micrometeorological measurement method.

6. Conclusions

When using studies published in the scientific literature to develop NH_3 emission factors for synthetic fertilizers for use in national emission inventories, the main factors to consider are the experimental approach, the chemical composition of the fertilizer, key environmental variables and the method of application. Methodologies for use in emission inventories need to account for the method of application, the chemical composition of the fertilizer and, for fertilizers not based on solid forms of urea, the interaction between the chemical composition and soil pH. Extending the methodology to account for the effect of the application rate of the fertilizer, and/or the effect of other variables such as the clay content of the soil and the air temperature might improve the accuracy of the inventory, depending on the extent to which these vary nationally. However, when extending a methodology to include these variables, it is important for the accuracy of the emission estimates and their value for use in policymaking that the input data is of a high quality.

In the models developed, the chemical, management and environmental variables account for a relatively small proportion of the variance in the emission data and this calls for more research and analysis for the causes of such weak relationships. Particular emphasis should also be placed on the assessment of measurement methods in two respects: a. the extent to which they can reliably and quantitatively measure *in situ* emissions from agricultural areas and b. whether lower cost, replicable small plot methods can be used to quantify relative emission reductions due to mitigation measures, even if they cannot be used to reliably quantify absolute emissions.

CRediT authorship contribution statement

N.J. Hutchings: Writing – review & editing, Writing – original draft, Project administration, Methodology, Data curation, Conceptualization. **J. Schoof:** Writing – review & editing, Data curation. **M. Mäenpää:** Writing – review & editing, Writing – original draft, Formal analysis. **A. Pacholski:** Writing – review & editing, Writing – original draft, Methodology, Conceptualization. **J. Webb:** Writing – review & editing, Writing – original draft, Methodology. **R. Albrektsen:** Data curation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jclepro.2025.147438.

Data availability

Data freely available from data repository with DOI (https://doi.org/10.3220/253-2025-14).

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