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AN INTERCOMPARISON OF MODELS USED TO SIMULATE THE ATMOSPHERIC DISPERSION OF AGRICULTURAL AMMONIA EMISSIONS

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Abstract: Ammonia emitted into the atmosphere from agricultural sources can have an impact on nearby sensitive ecosystems either through elevated ambient concentrations or dry/wet deposition to vegetation and soil surfaces. Short-range atmospheric dispersion models are often used to assess these potential impacts on semi-natural ecosystems and a range of different models are used for these assessments depending on the location and experience of the assessors. However, until now there has not been an intercomparison of the different models, for the case of ammonia dispersion from agricultural sources. This paper presents an intercomparison of some models commonly used for this type of assessment (ADMS; AERMOD; LADD and OPS-st). This intercomparison shows that there are significant differences between the concentration predictions of the models and some of these differences appear to be consistent and independent of the scenario modelled. In addition, the agreement between the model concentration predictions is dependent on source height with the models agreeing best for ground-level sources. The level of model agreement decreases with source height although the agreement between the three Gaussian models (ADMS, AERMOD and OPS-st) improves again as the source height increases to 20 m. When applied to two case study farms in Denmark and the USA model performance is 'acceptable' (i.e. the model predictions met most of the acceptability criteria) for all of the models except for the LADD model which is probably beyond its limits of applicability for one of the case studies (elevated source with a large exit velocity).

Key words: *Atmospheric dispersion models, evaluation, validation, ammonia, agriculture*

INTRODUCTION

Ammonia (NH_3) emitted into the atmosphere from agricultural sources can have an impact on nearby sensitive ecosystems either through elevated ambient concentrations or dry/wet deposition to vegetation and soil surfaces (Bobbink *et al.*, 1998). Environmental impact assessments are often carried out using short-range atmospheric dispersion models to estimate mean annual atmospheric concentrations and total annual deposition of NH_3 at the ecosystem location. A range of different atmospheric dispersion models are used for these assessments depending on the location and experience of the assessors and have not, until now, been compared for these types of assessments. For example, in the UK, modelling assessments for the dispersion and deposition of agricultural NH_3 emissions normally use one of two 'advanced' Gaussian dispersion models: ADMS (Carruthers *et al.*, 1994) or AERMOD (Cimorelli *et al*., 2002). In the USA, AERMOD is the recommended model, whereas in Denmark regulatory assessments are carried out using OML-DEP (advanced Gaussian; Sommer *et al.*, 2009), in the Netherlands, amongst others, OPS-st is used (advanced Gaussian; Van Jaarsveld, 2004; Van Pul *et al*, 2008) and in Germany the Lagrangian particle trajectory model AUSTAL2000 is used (Bahmann and Schmonsees, 2004). Assessments for research purposes have also been made in the UK using the LADD model (Lagrangian air column model; Hill, 1998).

There have been many attempts (see e.g. Hanna *et al.* (2001); Hall *et al.* (2001); Dunkerley *et al.* (2001)) to validate and intercompare the different models that are used for these assessments using industrial or research case studies (e.g. SO_2 and NO_x emitted by power generation plants or controlled tracer plume experiments) but very few of the studies have looked at dispersion of atmospheric NH_3 emitted by agricultural sources (Hill *et al.* (2001); Baumann-Stanzer *et al.* (2008)). Industrial sources tend to be elevated above ground, have small emitting areas and often the gases are emitted with high temperatures and exit velocities. In contrast, agricultural NH_3 emissions come mainly from animal housing and the storage and field-application of manures and slurries (Beusen *et al*., 2008) and are therefore emitted close to ground-level, at near-ambient temperatures, at low or zero exit velocities and often over large areas. The present paper compares four atmospheric dispersion models (ADMS 4.1, AERMOD v07026, OPS-st and LADD) for a series of hypothetical agricultural emission scenarios and evaluates the performance of these models using atmospheric NH_3 concentration data from two agricultural field experiments.

MATERIALS AND METHODS

Intercomparison of models for hypothetical scenarios

Four scenarios were used, representing typical source configurations for agricultural sources of NH_3 (Table 1).

Table 1: Source configurations used in the scenarios

Scenario	Source configuration	Representing
Sc1	Ground-level area source (20 x 20 m)	Slurry lagoon
Sc2	Elevated area source (20 x 20 m at height of 2 m above ground)	Slurry tank
Sc3	Volume source	Naturally ventilated livestock housing
Sc4	Line of 3 point sources (5 m above ground, 5 m separation, 0.5 m internal diameter, 5 m/s exit velocity, ambient temperature)	Artificially ventilated livestock housing

The domain used was 2 x 2 km square with roughness length, z0 = 0.1 m (to simulate agricultural land), with the NH_3 source in the centre. The meteorological dataset used was one year of continuous hourly data from the Lyneham meteorological station in the UK for 1995. These are the same data as those used by Hall *et al.* (2001) and are available pre-formatted for ADMS and AERMOD. The four scenarios were run for each of the models and simulated annual mean ground level (h=0.5 m) atmospheric NH_3 concentrations were compared for four horizontal transects (N, E, S and W) starting at the centre of the NH_3 source. Dry deposition was simulated by all models (using model-specific parameterisations for agricultural land cover) but wet deposition, terrain and building effects were not included in the simulations.

Model performance evaluation

For the assessment of model NH_3 concentration prediction accuracy, field measurements from two experiments were used. The first of these was by Pedersen *et al.* (2007), who made weekly measurements of mean atmospheric NH_3 concentrations at 27 locations around a pig farm in Falster (Denmark) during a period of three months. During the same period the NH_3 emission rate and meteorological data were measured hourly. The NH_3 concentrations measurements were made by exposing diffusion tubes at a height of 2 m above ground during 12 weekly periods. The pig house NH_3 emissions were calculated from NH_3 concentration measurements (by photoacoustic gas analyser) and air flow measurements in the 11 roof vents of the building.

The second dataset used was from Walker *et al.* (2008) who measured atmospheric NH_3 concentrations using diffusion tubes at a height of 1.5 m above ground around a pig farm in North Carolina (USA). Mean weekly concentrations were measured between June 2003 and July 2005 and a complete calendar year (2004) was used for the evaluation. No emission measurements were made for the main sources (5 naturally ventilated pig houses and a slurry lagoon) but annual NH_3 emission factors have been calculated for similar pig farms in North Carolina. In addition, hourly meteorological data were collected near to the farm.

Evaluation of model performance requires a statistical comparison of model predictions with observed values. Chang and Hanna (2004) summarise the indicators available for evaluating dispersion model performance. For the current evaluation, the five performance measures featured in the BOOT Statistical Model Evaluation Software Package (v2.0) have been used (Chang and Hanna, 2005). They are: fractional bias (*FB*), geometric mean bias (*MG*) normalised mean square error (*NMSE*), geometric variance (*VG*) and the fraction of model predictions within a factor of two of observations (*FAC2*). These performance measures relate the observed and predicted concentrations and their standard deviations.

FB and *MG* are measures of model bias (i.e. the tendency of the model to over or under predict concentrations), whereas *NMSE* and *VG* are measures of scatter in the predicted values relative to the observations and *FAC2* is a composite measure that takes into account both bias and scatter. Chang and Hannah (2005) suggest ranges for five of the performance measure values that indicate acceptable model performance. The ranges suggested are: $|FB|<0.3$, $0.7<MG<1.3$, $NMSE<1.5$, $VG<4$ and $FAC2>50\%$. Conclusions on model suitability were made by comparison of the performance measure values with these acceptability criteria.

RESULTS

Hypothetical scenarios

Modelled concentrations were output by the models along 4 transects (N, E, S and W). Due to the wind direction distribution in the meteorological data, the simulated concentrations varied greatly between transects and therefore, to simplify the intercomparison of simulated concentrations, a transect mean was calculated, which was the mean of the four transect estimates (N, E, S and W) for each distance from the source centre (Figure 1). The mean transect concentrations estimated by all models were similar for Sc1 (ground-level area source), although the rate of decrease with distance was greatest for ADMS and smallest for AERMOD (Figure 1a). Mean transect concentrations simulated by the models for Sc2 (elevated area source) were lower than in Sc1 and there was more variability between the models (Figure 1b). AERMOD estimated the largest concentrations along the entire transect, whilst the smallest values were estimated by LADD close to the source and by ADMS at distances greater than 800 m. For Sc3 (volume source), AERMOD predicted the largest concentrations and ADMS the smallest, although the differences between the models were not as great as in Sc2 (Figure 1c). Sc4 (3 elevated point sources) produced the largest variability between models, again with AERMOD predicting the largest concentrations and ADMS the smallest (Figure 1d). In general, close to the source, all models estimated a decrease in concentrations going from Sc1 to Sc4.

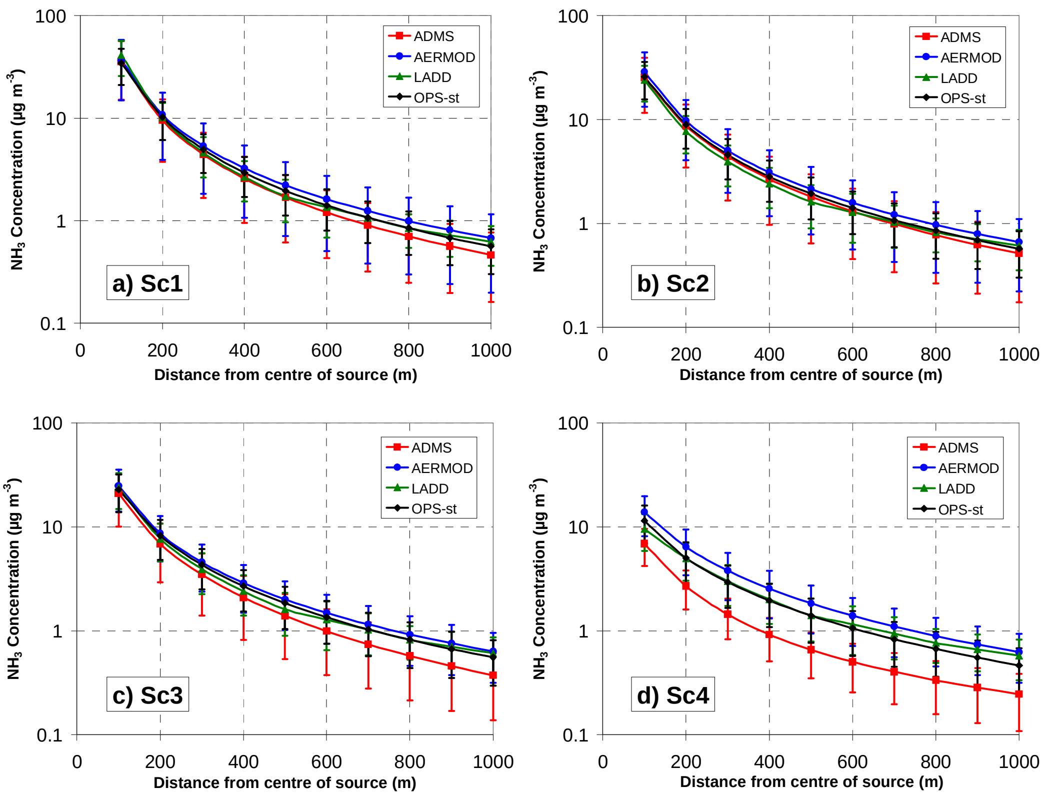

Figure 1: Mean transect (mean of N, E, S and W transects) concentration estimates for the four models evaluated for the four scenarios a) Sc1 (ground-level area source), b) Sc2 (elevated area source), c) Sc3 (volume source) and d) Sc4 (3 elevated point sources). Vertical bars represent ± standard deviation of the four transects at each distance. NB. The LADD model is unable to simulate scenario Sc3 and therefore the profile transect from Sc2 is shown for comparison.

Model performance analyses

Figure 2a shows the comparison between the mean measured concentrations and those predicted by the four models for the Danish case study (Falster) over the three month measurement period. The three regulatory models (ADMS, AERMOD and OPS-st) produce similar predictions with OPS-st, in general, predicting higher concentrations than AERMOD, which in turn predicts higher values than ADMS. The LADD model on the other hand predicted much larger concentrations than the other three models. AERMOD meets the model acceptance criteria for all performance measures and ADMS and OPS-st meet all but one of them (*FB* and *MG* respectively). LADD only met one of the acceptance criteria (*NMSE*) for this case study. Another dispersion model, OML-DEP (Sommer *et al.*, 2009), was also evaluated for this case study by Pedersen *et al.* (2007) and an analysis of the performance measures shows that this model meets all but one of the acceptance criteria (*MG*). Figure 2b shows the comparison between the mean measured concentrations and those predicted by the four models for the USA case study (North Carolina) over a one year measurement period (2004). In general, all of the models overestimate the measured concentrations, with the largest overestimate from the OPS-st model followed by AERMOD. From the values of the performance indicators, only LADD and ADMS met all of the acceptability criteria with AERMOD and OPS-st not meeting the bias criteria (*FB* and *MG*) due to over prediction.

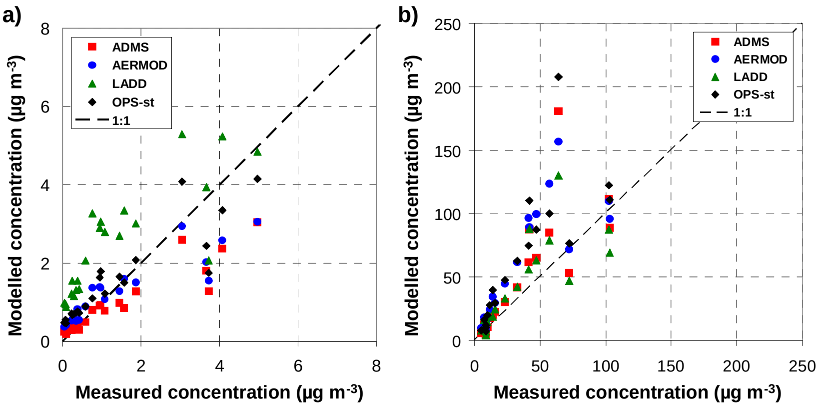

Figure 2: Modelled versus measured atmospheric ammonia concentrations for a) the Danish pig farm and b) the USA pig farm.

DISCUSSION

Why do the model estimates differ?

An analysis of the hypothetical scenarios allows us to look at why the models give different concentration estimates for different source types. All models gave similar concentration estimates for Sc1 (ground-level area source) suggesting a robustness in model predictions for these types of sources. For Sc4 (elevated point sources), however, larger variations between models were present, which warrants a more detailed investigation. Re-running Sc4 with a range of source heights (0, 2, 5, 10, 15 and 20 m) and with zero exit velocity shows that the agreement between the models depends strongly on the source height. Figure 3 shows the mean estimated concentration across the domain for a 100 x 100 grid of receptors (h= 0.5 m) for each model and each source height. With a ground level source all mean model estimates are within 20% of each other but as the source height increases to 5 m, there are larger differences between the model estimates (up to 50%). Including a 5 m s^{-1} exit velocity in the ADMS and AERMOD simulations increases this difference further (to more than 100%), which is in agreement with the mean transects from Sc4. The models continue to disagree as the source height increases further although the mean concentration estimates of the three Gaussian models (ADMS, AERMOD and OPS-st) become closer at a source height of 20 m. At this height LADD estimates the mean concentration to be approximately twice that of the other models. LADD was designed for use with ground or low-level agricultural sources. The model assumes a constant wind speed with height, which is a valid approximation for dispersion close to the ground but this approximation ceases to be valid for elevated sources, resulting in over-estimation of ground-level concentrations. A comparison of the three Gaussian models shows that ADMS and OPS-st predict very similar mean concentrations for source heights above ground level. AERMOD, on the other hand, predicts a higher mean concentration for these sources except for a source height of 20 m, for which the model predicts a similar mean concentration to the other two Gaussian models.

These analyses can explain some of the differences encountered in the model performance evaluation. For the Danish case study the source height was 6.4 m and the mean exit velocity was 8.2 m s^{-1}. This exit velocity will significantly reduce the concentration predictions for ADMS and AERMOD compared with those of LADD and OPS-st (which cannot simulate exit velocities). This is a similar situation to the 5 m source height simulation of Figure 3 but with an increased reduction in the mean concentration predictions of ADMS and AERMOD due to the larger exit velocity. This may explain why, in general, LADD predicts the highest concentrations followed by AERMOD and OPS-st with ADMS predicting the lowest concentrations for this case study. The USA case study simulations used source heights of 0 m for the slurry lagoon and between 0 and 2.5 m for the pig houses (depending on how they are represented in the models). For this case study, in general, OPS-st and AERMOD predicted the highest concentrations and ADMS and LADD the lowest. This is similar to the situation shown in Figure 1c (Sc3) for a volume source, which is the source type used for the main source in this case study (naturally ventilated pig houses). Although these analyses do not investigate the reasons for differences between the model predictions (since this would require a detailed study of the model dispersion parameters), they do highlight the types of assessments which would give the largest differences in concentration predictions.

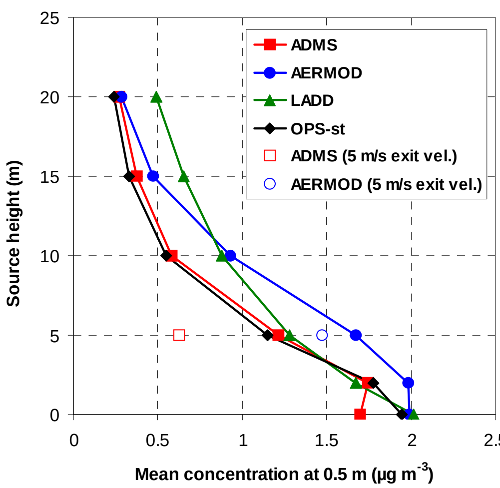

Figure 3: The dependence on source height of the mean ammonia concentration predictions for the four models for a 100 x 100 grid of receptors (h=0.5 m).

Are the models acceptable for assessments?

Although it's difficult to make firm conclusions on model acceptability from just two case studies, the performance evaluation provides further evidence of model suitability that can be added to the conclusions of past and future validation studies. Most of the models meet the majority of the criteria for both case studies suggesting that the models are acceptable for these types of simulations. Uncertainty in model inputs such as emission rates for the USA case study could easily account for models missing some of the criteria. The only exception is the LADD simulation of the Danish case study, which only met one of the acceptability criteria. This simulation is on the limit of applicability of the LADD model, which was designed for ground- or low-level sources, not roof vents with large exit velocities and it is concluded that this model is probably not suitable for simulations with sources above heights of 5 m with large exit velocities.

CONCLUSIONS

This paper provides a comparison and evaluation of four models commonly used to simulate the atmospheric dispersion of ammonia emitted by agricultural sources. A hypothetical study using different source configurations shows that model concentration estimates are similar for ground-level sources but the discrepancies between model estimates increase with source height, although the three Gaussian models (ADMS, AERMOD and OPS-st) begin to agree more as the source height is increased to 20 m. A statistical model performance analysis using mean atmospheric ammonia concentrations measured in two experiments show that all models perform 'acceptably', with the exception of the LADD model that is probably not suitable for the simulation of one of the case studies (source height in excess of 5 m with large exit velocities).

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