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EXTENDED ABSTRACT

Abstract title: Estimating concentration and deposition of ammonia and nitrogen oxides at the local scale: an intercomparison of eight operational models

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Introduction

Deposition of reactive nitrogen species on natural ecosystems can have negative effects on environmental quality and biodiversity. This nitrogen comes from different sources such as traffic, agriculture and industry. Estimates of nitrogen deposition are used for policy advice and permitting of economic activities. The Dutch government has initiated a research program that aims to improve the national reactive nitrogen modelling and measurement strategy. As part of this research programme, a benchmarking exercise was carried out to intercompare computed local scale concentration and deposition from commonly used atmospheric dispersion and deposition models for different sources and land cover types (Kooi et al. 2025). Key results include the extent to which period-average concentrations and deposition fluxes differ among models, and an identification of the meteorological conditions that most influence these discrepancies. A comparison with measurements was carried out in a companion study (Thorkelsdottir et al. 2025).

Methods

Concentration and deposition outcomes from eight atmospheric dispersion and deposition models were intercompared for four source types. The included source types are livestock housing (NH_3), manure application (NH_3), a tall buoyant industrial stack (NO_x) and motorway traffic (NO_x). Receptors were placed at seven distances from the source (ranging from 50 m to 5 km) and in twelve directions. The selected models (ADMS, AERMOD, IFDM, OML-Multi, OPS-ST, OPS-LT, SRM2 and STACKS-D)[1] are all used for air quality and deposition calculations on a local scale, for regulatory and other applications. Corresponding emission characteristics were defined by RIVM. Simulations were performed for three different types of land cover: homogeneous grass, homogeneous

[1] SRM2 was only used for the motorway case and OML-Multi was not used for that case.

forest, and realistic heterogeneous land cover. The simulations covered a 10-year period: 2011-2020, and used meteorological observations from the Royal Netherlands Meteorological Institute for a central location in The Netherlands.

The primary aim of the study was to examine the extent of differences between models and to identify conditions under which these differences are most pronounced. Model comparisons were based on annual average concentrations and ten-year average deposition fluxes. The latter restriction was due to a limitation in the available output from one of the models. For models that provided hourly outputs, the meteorological conditions relating to the largest inter-model differences were identified.

Several options to quantify the extent of differences were explored. The Geometric Standard Deviation (GSD) was identified to be the most useful metric out of the range of metrics considered. In broad terms, the GSD quantifies the typical deviation factor of model outcomes relative to their Geometric Mean (GM) outcome[2]. GSD is particularly useful when outcomes are bounded by a minimum (e.g. 0) and if the variance between outcomes is significant[3].

In order to explore the relevance of atmospheric stability on outcomes, hourly calculated values of the Monin-Obukhov length (L) from OPS were used to classify hourly meteorological conditions into nine stability classes, ranging from extremely unstable, via neutral, to extremely stable. The classification basically follows (Gryning et al. 2007), but has two additional classes: extremely unstable ($-50 \le L < 0$) and extremely stable ($0 < L \le 10$) weather conditions.

Results

Concentration and deposition outcomes

Figure 1 shows average concentrations from individual models for different distances and source types over realistic land cover (top), and the extent of differences in model outcomes in terms of GSD (bottom). Concentrations rapidly decline with distance, although for the tall industrial stack only downwind of where the plume impacts the ground. The smaller reduction with distance for the motorway is primarily due to the different source topology (line source versus point source). The GSD, which measures the extent of differences in model outcomes, is mostly between 1.5 and 2. Larger values of GSD are found very close to the farm building (at 10 m from a side of the building), close to the industrial stack (where models disagree in terms of how fast elevated buoyant plumes impact the ground) and for the largest distances from sources with emissions of ammonia. The latter is partly the result of one of the models not accounting for source depletion in concentration calculations. The variance of GSD at a specific distance mostly reflects variance in direction, not between years.[4]

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[2] The following formulae apply: $GSD = exp\sqrt{\frac{1}{n-1} \cdot \sum_{i=1}^{n} \left(\ln\left(\frac{M_i}{GM}\right)\right)^2}$ and $GM = exp\left[\frac{1}{n} \cdot \sum_{i=1}^{n} \ln\left(M_i\right)\right]$.

[3] If a distribution of outcomes is lognormal, 68% of all outcomes is within 1 GSD distance from the GM.

[4] This is relevant when comparing GSD for annual concentrations with GSD for 10-year average deposition.

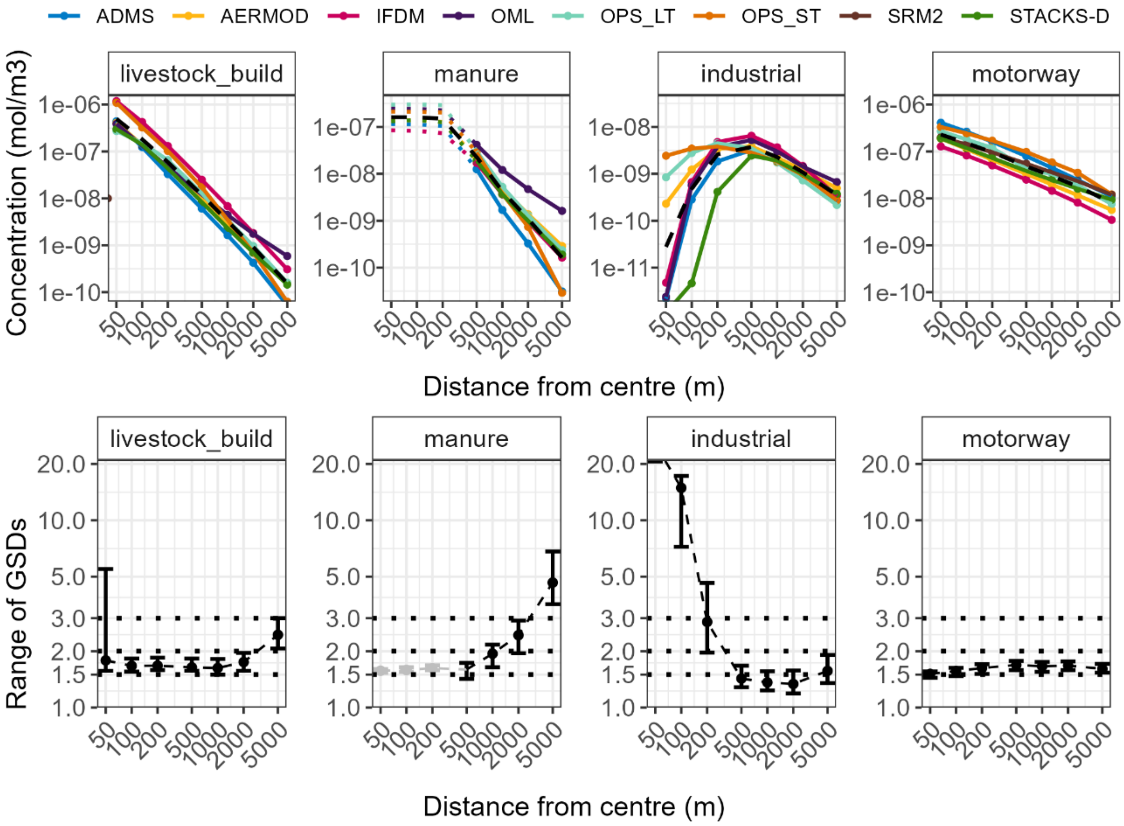

Figure 1 Individual model outcomes for average annual concentrations (top) and extent of differences in model outcomes in terms of GSD (bottom), for the different source types over a realistic heterogeneous land cover. The 'error' bars (bottom) indicate the range from the 5th to the 95th percentile in a set of 120 outcomes (10 years and twelve directions). Horizontal and vertical axes are logarithmic.

Figure 2 shows results for 10-year average deposition fluxes. The trend with distance (top) is similar to that for (annual) concentration outcomes (Figure 1), indicating a strong correlation between calculated concentrations and deposition fluxes as expected. Differences in modelled deposition in terms of GSD are now mostly between 2 and 3. Significantly larger GSD values close to the livestock farm and the industrial stack relate to the large range of ground-level concentrations at these locations. GSD's for the two ammonia cases increase less rapidly with distance than for concentrations (Figure 1), in part because the model that did not apply source depletion to concentrations does so for deposition.

<u>Impact of atmospheric stability</u>

Hourly concentrations were provided by five models (ADMS, AERMOD, IFDM, OML and OPS-ST). Atmospheric stability was particularly relevant for identifying when model outcomes differ substantially. Hours with extremely or very stable weather conditions contribute the most to the annual average concentrations for sources with a low emission height (livestock housing, manure application and motorway). The largest differences between models also occur in these weather conditions. Similar findings have previously been reported in (Theobald et al. 2012). For the industrial stack, hours of extreme or highly unstable weather conditions contribute the most to short-range concentrations (up to and including 200 m), while hours with stable weather conditions become increasingly important from 500 m onwards. The largest differences between models again occur during the aforementioned weather conditions. Hourly deposition fluxes were only generated by three models (ADMS, AERMOD and OPS-ST), and showed similar patterns as for concentrations, although slightly less prominent.

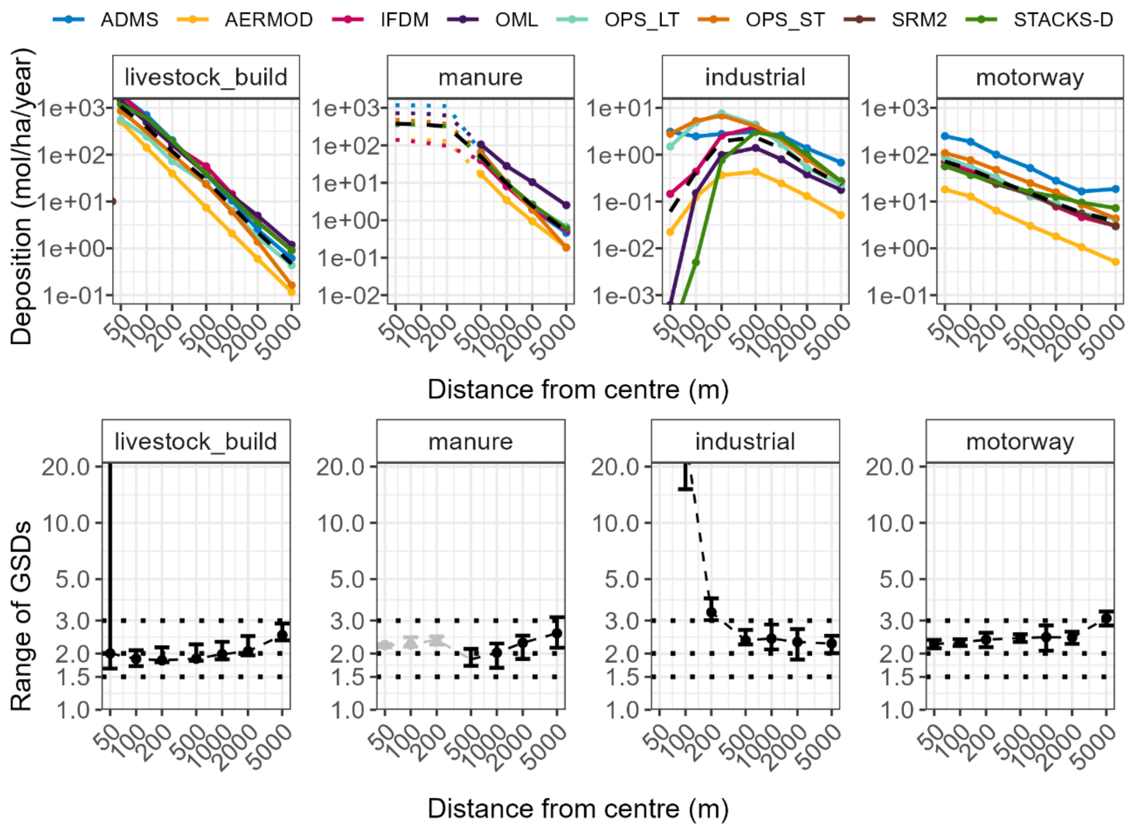

Figure 2 Individual model outcomes for 10-year average deposition (top) and extent of differences in model outcomes in terms of GSD (bottom), for the different source types over a realistic heterogeneous land cover. The 'error' bars (bottom) indicate the range from the 5th to the 95th percentile in a set of 12 outcomes (twelve directions). Horizontal and vertical axes are logarithmic.

Discussion and conclusions

The model intercomparison showed similarities and differences between the selected models. Similarities include relative trends of concentrations and deposition fluxes with distance, strong correlations between calculated concentrations and deposition fluxes, relative effects of land cover on concentrations and deposition (not shown in this paper), and the large contribution of very stable weather conditions to annual concentrations and deposition, in particular related to sources with low emission height. Differences between model outcomes are expected to be the result of differences in the processing of meteorological parameters and different model formulations for plume rise, dispersion and deposition. The largest absolute differences in annual-average model outcomes mostly relate to hours with very stable weather conditions. Hours with very unstable weather conditions are important to inter-model differences close to the tall buoyant stack. A detailed understanding of the exact causes of model differences requires access to internal model parameters, such as micrometeorological parameters, plume height, dispersion coefficients and deposition velocities.

Differences among model outcomes were expressed in terms of the Geometric Standard Deviation. GSD’s for concentration were mostly between 1.5 and 2 for annual concentrations in different years and directions and between 2 and 3 for 10-year average deposition in different directions. The largest GSD’s were found at 10 m distance from the sides of the farm building and relatively close to the industrial stack (up to 500 m). The latter is a result of different predictions of how quickly the elevated plume impacts the ground. Differences in deposition outcomes are the result of different predictions of ground-level concentrations and different effective deposition velocity modelling approaches. Model differences can be reduced by harmonising the processing of meteorological parameters, harmonising dispersion in very stable weather conditions and harmonising formulations for deposition processes.

This intercomparison of model outcomes does not identify which models perform better or worse. However, a comparison with measurements was carried out in a companion study (Thorkelsdottir et al. 2025).

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