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IMPROVING HIGH RESOLUTION URBAN CONCENTRATION MAPS THROUGH MODEL HARMONIZATION AND INVERSE MODELLING

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Abstract: Each year, the RIVM publishes maps of annually averaged concentrations for the Netherlands for the major atmospheric pollutants on a scale of 1x1 km. These maps are produced with the OPS-LT model and are broadly used as background concentration maps in the Netherlands. For urban applications, however, local authorities require higher resolution maps to accurately assess the exposure of urban citizens to atmospheric pollutants.
In this study we use a large dataset of urban NO_2 measurements by passive samplers to validate high resolution maps, to evaluate potential model improvements and to identify remaining short comings of the model. The OPS-LT model was run at a resolution of 250x250m for the regions of Utrecht, Amsterdam and Rijnmond. Changes to the model were made by harmonizing the chemistry and emission characteristics with the extensively validated Dutch road traffic model, SRM2. Finally, through inverse modelling (Bayesian inference), model results and measurements were combined to obtain a detailed overview of emission sector specific biases.
We found that the increase in spatial resolution yielded a limited improvement of the model performance, but that the model harmonization did improve performance on all validation datasets. Inverse modelling suggests potential biases in the contributions from shipping and foreign sources.
Our results show that large datasets of urban measurements are key in validating potential model improvements. Provided that such datasets are large enough, inverse modelling techniques can be used to obtain detailed insights in model biases. These insights can be used to prioritize research in emissions to obtain better estimates of emission sector contributions to the exposure of urban citizens to atmospheric pollutants.

Key words: *Urban modelling, model harmonization, high resolution modelling, Bayesian statistics, inverse modelling.*

INTRODUCTION

Annually, large scale concentration maps for The Netherlands (referred to as GCN maps) are published by the National Institute of Public Health and Environment (RIVM). These maps are calculated using the Operational Priority Substances (OPS-LT) model with a resolution of 1 by 1 kilometer, adequate for background mapping (Hoogerbrugge et al., 2023, Sauter et al., 2023). Higher resolution calculations are performed separately with different models, and added to the GCN background maps to identify local hotspots, particularly near roads.
Apart from identifying such legal hotspots, there is a growing need to map exposure to air pollution. At the same time, the dominance of traffic contributions to air pollution is diminishing, meaning that exposure becomes a complex mix of different emission sector contributions. In this study we explore the possibility of creating GCN maps by calculating contributions from all sectors separately at higher resolutions.

In addition to mapping local exposure, it is crucial for policymakers to have insights into the origin of air pollution. Regular GCN maps consist of separate OPS calculations for different emission sectors. The quality of these calculated sectoral contributions can only be assessed by comparing the sum of these contributions (i.e. the background map) with measurements. A good agreement with measured concentrations indicates accurate calculation of individual sectoral contributions.
In this study we employ a large set of passive NO_2 samplers (Palmes tubes) to assess how well the calculated concentrations compare with measured concentrations in urban areas. We do this using the standard OPS configuration and after adjusting some model settings. Furthermore, we explore the possibility of combining the vast amount of available measurements with Bayesian statistics to detect potential biases in sectoral contributions.

CALCULATIONS AT HIGHER RESOLUTION

For this research, we conducted OPS calculations with the NO_x emissions determined by the Dutch Emission Registration (ER) at a resolution of 1 by 1 kilometer and with higher resolution emissions at 250 by 250 meters. Calculating a map of concentrations for the entire Netherlands at an increased resolution of 250 by 250 meters would take approximately 256 (or 16 times 16) times longer than regular 1 by 1 km calculations. Therefore, we chose to only increase the resolution of sources in a selection of urban areas, as a significant portion of emissions and exposure occurs here. Additionally, we currently calculate only at measurement locations, not at locations without measurements.
We selected three areas with many NO_2 measurements: the Rijnmond region, the Utrecht region, and the Amsterdam region. All regions were calculated using emissions and meteorology from the year 2019. For this year, many measurements are available, especially in the Rijnmond region (at about 230 locations; Van Breugel & Van den Elshout, 2020).
The calculated and measured annual average NO_2 concentrations are compared in Figure 1 for the Rijnmond region. The figure shows that the increase in resolution gives a limited improvement in model performance. The calculations for the Utrecht and Amsterdam regions show similar minor improvements.

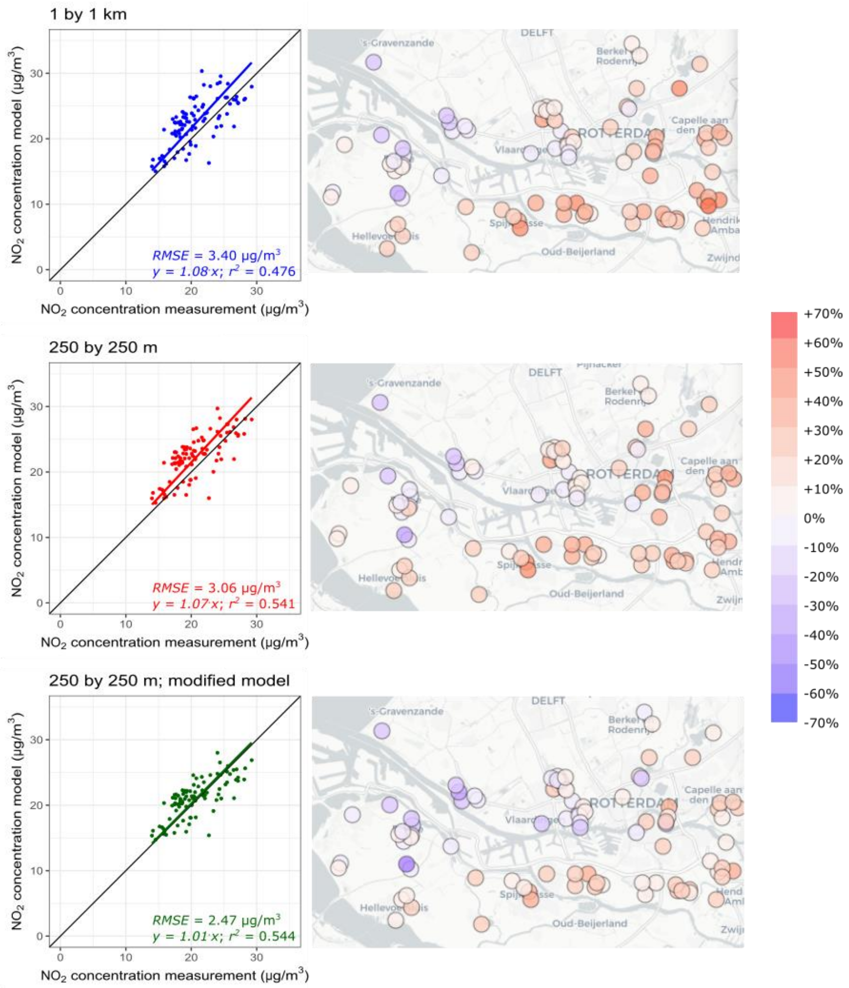

Figure 1. Comparisons between model and measurement for the Rijnmond region. Left: scatterplots of model versus measurement, with some performance metrics. Right: maps of the relative difference between model and measurement. Top: calculations with emissions at 1 by 1 km, center: calculations with emissions at a higher resolution of 250 by 250 m, bottom: calculations with a modified version of OPS with emissions at a resolution of 250 by 250 m.

MODEL ADJUSTMENTS

In addition to refined calculations, we conducted calculations with a modified version of the OPS model; these modifications are described below. The model adjustments are largely inspired by Standard Calculation Method 2 (SRM2). This model has long been used in the Netherlands to calculate local traffic contributions at high resolution and has also been extensively validated with measurements (Wesseling et al., 2020).

NO_2 chemistry

The OPS model only outputs NO_x concentrations. To determine NO_2 background concentrations, a relationship between NO_2 and NO_x, derived from measurements at background locations of the National Air Quality Monitoring Network (luchtmeetnet.nl; the black line in Figure 2) is used to obtain regular GCN NO_2 maps. This relationship works well at background locations, but near sources, NO_2 concentrations can be overestimated. This can be seen in the difference between the blue points and the black line in Figure 2. In the modified version of OPS, we adopted the NO_2 chemistry from SRM2 (Wesseling & Van Velze, 2014). This treatment of NO_2 chemistry can theoretically be applied to all types of sources, but has primarily been validated for road traffic sources. Therefore, we only apply the adjusted chemistry to road traffic sources.

Calculation at measuring height
Near sources, the OPS model calculates concentrations only at the surface. To also calculate concentrations at higher altitudes, we adapted the OPS model to calculate the concentration at a user-specified height. This allows for better comparison with measurements. The passive samplers are often placed on lampposts at 2 to 3 meters high, but citizen measurements in the Rijnmond region are sometimes done at greater heights, in apartment buildings.

Capping of meteorological input
The validity of assumptions in air quality models are sometimes limited to a certain range of meteorological input. In addition, some meteorological variables cannot be accurately determined below a certain threshold value (=detection limit). Therefore, many air quality models cap the meteorological input. Above or below a threshold value, the variable's value is assumed to be equal to the threshold value. For the SRM2 model, this capping is performed in a preprocessing tool called preSRM. The threshold values in our modified version of OPS are set equal to those of preSRM.

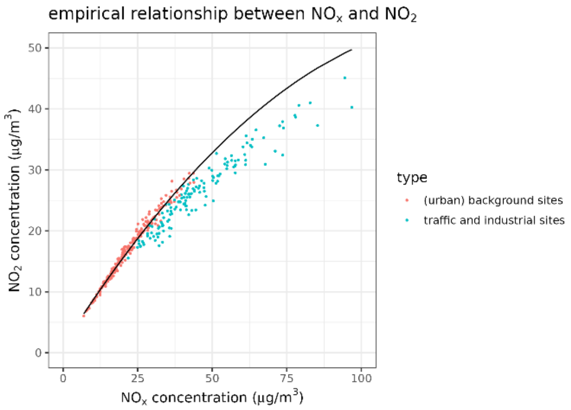

Figure 2. The empirical relationship (black line) between NO_2 and NO_x used for regular GCN maps to convert the NO_x concentrations calculated by OPS into NO_2 concentrations. This relationship works well at (urban) background locations (red points) but not at traffic and industrial measurement sites (blue points).

CALCULATIONS WITH THE MODIFIED OPS MODEL
Figure 2 shows the effect of the combined model adjustments on model performance for the Rijnmond region. The original OPS calculations show a systematic overestimation in city centers (red dots on the map). This overestimation decreases with the model adjustments. We also observe spatial patterns in the difference between the model and measurements. For example, in the center of Rotterdam and Amsterdam, we see overestimations by the model, while along waterways, the model underestimates the NO_2 concentrations. Such spatial patterns can contain information about biases in the sectoral contributions to air quality. For example, the underestimation of concentrations near waterways may indicate underestimation of the contribution of the shipping sector to air quality.

STATISTICAL ANALYSIS OF SECTORAL CONTRIBUTIONS
With the large quantity of measurements now available for some urban regions, we can do more than just scatter plots and maps. Through a statistical method called Bayesian inference, we can assess the quality of the calculated sectoral contributions to concentrations.
An initial assessment of the quality of the modelled sector contributions follows from the reported uncertainties in ER emission totals (Wever et al., 2023). Figure 3 shows what the probability distributions based on these uncertainties look like (red; termed 'a priori'). We can then add information in the form of measurements. Including measurements changes the probability distributions: they become wider or narrower and/or shift to higher or lower contributions. These adjusted probability distributions are shown in blue ('a posteriori').

The shifting of the probability distributions indicates that the calculated contributions deviate from the actual sectoral contribution. In all three regions studied, we see a shift of the probability distributions for the traffic and other traffic sectors towards lower concentration contributions. For the shipping and fisheries sector, we see a shift towards higher contributions for the Rijnmond region (Figure 4) and the Amsterdam region. Finally we observe that sectors that show no clear spatial differences in concentration contributions and also have large 'a priori' uncertainties, such as foreign emissions, are significantly adjusted in our analysis. This seems to be a weakness of our analysis because the results for such sectors are often inconsistent. For example, the contribution from foreign sources shifts towards lower contributions for the regions of Utrecht and Rijnmond, and remains the same for the region of Amsterdam.

Note that deviations from the sectoral contributions reported in GCN, as shown in Figure 4, can have various causes. The deviations can be caused by uncertainties in emissions, but uncertainties in emission characteristics (source height, heat content of emissions, etc.) and uncertainties in modeling also influence the modeled sectoral contributions. A shift in probability distributions therefore does not immediately mean that we need to adjust emissions, but it can provide direction for research into emissions and emission characteristics.

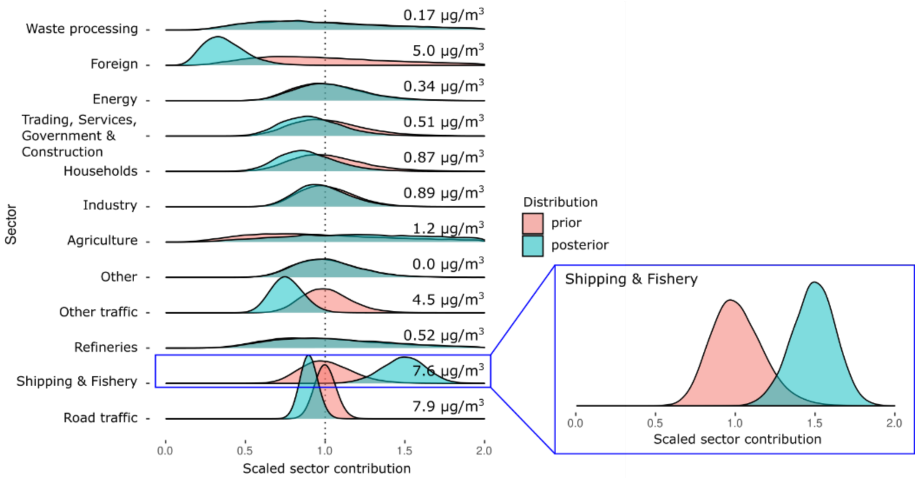

Figure 3. Probability distributions of sectoral contributions at the measurement sites for the Rijnmond region, before (red) and after (blue) adding the measurements. All probability distributions are scaled so that a value of one represents the sectoral contribution as would be found in a regular GCN map. The displayed concentration contributions are the averages over all measurement locations in the Rijnmond region before scaling. The runs were conducted with emissions at 250 by 250 meters, using the modified OPS version. The modified NO_2 chemistry could not be included in this analysis, due to non-linearities.

CONCLUSION

In this article, we explored how to calculate exposure to and origin of air pollution in the city in more detail and with higher accuracy. We conducted calculations with sources at higher resolution and after implementing some model adjustments. We compared these calculations with NO_2 measurements in urban areas. Additionally, we employed statistical analyses to use the same measurements for a better estimation of the origin of air pollution and to detect potential biases of sectoral contributions.

We found that higher resolution of emission input does not necessarily provide a significant improvement in concentration calculations for urban areas. However, the implemented model modifications did result in clear improvements. With our statistical analysis, we can identify sectors where we need to conduct more research in the future.

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