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DEVELOPING A METHOD FOR HIGH-RESOLUTION ANNUAL CONCENTRATION ASSESSMENT AND SCENARIO ANALYSIS FOR NO_2 FOR THE WHOLE OF EUROPE

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Abstract: In this contribution we present a fast method to estimate the annual NO_2-concentrations for the whole of Europe at a resolution of 125m. In order to do so in a reasonable amount of time, we apply a dispersion kernel method applied to the major source of local NO_2-concentration gradients in Europe : road traffic. In this method, a list of NO_x dispersion kernels is pre-calculated using the IFDM Gaussian dispersion model for the different weather regimes in Europe across different road directions, leading to a database of standard patterns of NO_x-concentration fields for line sources with a fixed unity emission. These kernels are then applied throughout Europe, multiplying the results with the effective emissions of each of the road segments. The latter are estimated using a downscaling of the 7x7 km² EC4MACS NOx-emission dataset onto the major roads, taken from Open Street Maps. The resulting NO_x-concentrations are combined, including corrections for double counting, with the results of a NO_2-CHIMERE simulation for the year 2010, using a parametric annual averaged NO_2/NO_x chemistry scheme adapted from Düring et al. (2011). Comparing to the CHIMERE (7x7 km²) background map, the 125m-resolution map reduces the bias from -28% to -19%, decreases the RMSE from 56% to 50%, increases the R^2 from 0.34 to 0.43 and increases the slope of the orthogonal regression from 0.96 to 1.11 with respect to the NO_2 concentrations measured at monitoring stations (Airbase). Our map complies with the FAIRMODE MQO for 68% of all stations, compared to 61% for CHIMERE. These results are obtained in an calculation time of about 3h on 24 CPUs (each using 6 threads).

Key words: *NO_2-modelling, kernel methods, fast modelling.*

INTRODUCTION

In this contribution, we propose a method to assess the NO_2-concentrations across all of Europe, striving for the following specifications:

1. A resolution of minimally 1km, with an ultimate goal of a resolution of about 100m.
2. The methodology should allow for the calculation of scenarios, meaning that the methodology should return a change in concentration (or exposure) in a deterministic, well defined way following a change in emission.
3. The method should have a limited calculation time (in the orders of at maximum some days walltime), in order to avoid excessive computational needs.
4. The method should improve the accuracy of the concentration pattern compared to the current CTM-based maps.

Within the epidemiology community, the use of so-called land use regression (LUR) models is widely established to derive population exposure in cohort studies (Beelen et al., 2013). Even though dispersion models and LUR are both adequate methodologies for NO_2-assessment (de Hoogh et al., 2014), LUR models cannot reliably be used for scenario calculation. For each proxy parameter, they derive regression coefficients from the correlation between a set of land use/land cover based proxy data and observations of NO_2 concentrations, . In a scenario context, these coefficients would be interpreted as a sensitivity with respect to the emissions assigned to that particular proxy. However, due to the high degree of correlation often found between different proxy parameters, the assignment of these sensitivities is not embedded in the fitting of the model in a fully deterministic way, making the interpretation of the regression weights problematic. LURs are therefore considered to be restricted to the time period and geographical area of the monitoring campaign (de Hoogh et al., 2014) used for their creation.

We propose a dispersion kernel-based methodology as the way forward, because this combines the causal relationship between emissions and concentrations found in dispersion modelling with a fast computation time (via the usage of kernels). In the next section we elaborate and describe this methodology attempting to deploy it at 100/125m resolution EU-wide.

METHODOLOGY

General

The methodology is based on a "bottom up" approach. Starting from coarse resolution background concentration grids (in which we assume all relevant emissions are represented), the emissions for the sectors of interest (i.e. SNAP7, road traffic) are replaced by a higher resolution dispersion calculation, explicitly accounting for individual point or line emission sources. This method is described in detail in the scientific literature (e.g. Lefebvre et al., 2013).

The objective is to explicitly factor in traffic emissions (SNAP7) , being the dominant source sector for NO_2 concentrations, at the level of line sources. This allows the increase of spatial resolution to an unprecedented level and enables traffic emission scenario calculations at these spatial scales. In addition, further refining the methodology when more detailed traffic information is released becomes an option. Assuming that traffic emissions can be adequately attributed to line sources, air quality assessment usually use a local scale dispersion model, often based on Gaussian or Lagrangian principles, to generate the resulting concentration pattern. However, a complete hour-by-hour calculation using such a model is unfeasible at EU-scale. Hence, an alternative approach is required.
We are mainly interested in the annual averaged concentration levels, so the idea is to make use as much as possible of pre-computed dispersion patterns that reflect the annual averaged dispersion characteristics at a specific location in Europe. Afterwards, the dispersion patterns or so called "kernels" can then be scaled with the particular emissions of a specific line source and integrated in an overall air quality map that takes into account all relevant sources in the area. This method is referred to as the "kernel method" in which a database of such dispersion patterns or kernels is produced in pre-processing.

Kernels

By definition dispersion kernels are being pre-computed for a set of 'standard sources'. As traffic is the main sector of interest in this study, the standard sources are line sources, i.e., roads. We have chosen line sources of 100m lengths at varying angles from the North-South axis in steps of 5°, thus 18 possible line segments in total. For every relevant region in Europe, using the relevant meteorological pattern for the year 2015, the annual mean NO_2 concentration patterns belonging to these 18 standard sources, using a standard unit emission strength of 1 kg/km/h, have been calculated and are stored in a kernel database. The dispersion simulation for such a standard line source is performed for a square area of 4x4 km² with the source centre in the middle. It is assumed that beyond the distance of 4km the impact of an individual line segment of 100m can be neglected and disappears into the regional background. The kernel simulations are performed at a resolution of 25x25m² using ECMWF meteorology. For the calculation of the kernel dispersion patterns, the IFDM (Immission Frequency Distribution Model, http://pandora.meng.auth.gr/mds/showlong.php?id=50) Gaussian dispersion model was used (Lefebvre et al., 2011, 2013).
It is important to state that even though this methodology was implemented and tested using the IFDM dispersion model, the choice of the dispersion model is not an essential part of the methodology and could be replaced by other local scale Gaussian or Lagrangian dispersion models.

The used reference road database was constructed based on the open transport map dataset (http://opentransportmap.info/). Only roads larger or equal to *SecondClass* roads were taken into account. First of all, the road segments were simplified with a maximum tolerance of 25m and split at the vertices to have straight line segments. The line source geometries were re-projected to the EU-wide INSPIRE coordinate system in which the tool is developed (EPSG: 3035) intersected with the background map grid and the meteorology grid, and the coordinates of the beginning and ending of the line segments were attributed to each line segment. Next, the SNAP 7 sector emissions are distributed along these line sources, so that the sum of the line source emissions for every 7x7 km² cell, is equal to the total for the

SNAP 7 sector for that cell. In order to do this, a proxy for the distribution of the road emissions has to be defined. We have chosen to use the 'road **capacity*length in grid cell**' as a proxy for this ratio. Note that as a result of the methodology, the proxy is only used to spread emissions **within** the 7x7 km^2 emission cells, not in between different cells.

Creation of the European-wide map

First, an EU wide high resolution grid at 100x100m² is constructed. For each 100x100m² grid cell, two variables are defined and initialized to 0. These variables will track the concentrations for NO_x (`C_NOx`) and for NO_2 (`C_NO2`) as passive pollutants during the calculations.

The database of line sources as defined above is split into line segments of 100m and according to its location and orientation each segment is connected to the specific kernel as defined above. In the next step, for every of those road segments, the contribution of the corresponding kernel grid (4x4 km² at a 25x25m² resolution) towards the European grid is derived. A loop over the relevant 100m grid cells is performed and for each of those grid cells `C_NOx` and `C_NO2` are calculated as follows (for all grid cells which receive a contribution of the line source under investigation):

```
C_NOx = C_NOx + E*kernel                (1)
C_NO2 = C_NO2 + E*R*kernel              (2)
```

Where *kernel* is an average over the 25m kernel cells that cover the 100x100m² grid cells, *E* is the emission of the line source in kg/km/hour, and *R* is the NO_2 over NO_x emission ratio. At the end of this procedure, the 2D-arrays `C_NOx` and `C_NO2` contain the concentrations of NO_x and NO_2 as if both were passive pollutants (no chemistry at the moment) and if no background concentrations of NO_x and NO_2 were present.

Next we treat the background concentrations. However, in doing so, a double counting of emissions should be avoided. Double counting arises because the traffic emissions are present both in the regional background model as well as in the high resolution kernel results. To avoid this double counting, we average the local contribution over the background cell and subtract this result from the background before adding the local contributions at high resolution. This is similar to what has been done in Lefebvre et al. (2013).

Until this point, no chemical interaction is taken into account between NO_x and NO_2.The latter one is the result of background contributions or directly emitted NO_2. To account for the chemical equilibrium in the atmosphere we rely on a procedure similar to the one described in (Düring et al., 2011).

Result and validation

Calculation of the EU-wide kernel based NO_2 map took about 3h on 24 CPUs (6 threads per CPU). Note that the application of the kernel method can easily be parallelized using domain decomposition, i.e. splitting the domain spatially for the calculations and stitching it back together afterwards. The calculation was initially performed at a resolution of 100m, whereas the final gridding was aggregated to a resolution of 125m in order to avoid data gaps in the final map.

A visual comparison of the CHIMERE background map with the AIRBASE (https://www.eea.europa.eu/data-and-maps/data/airbase-the-european-air-quality-database-7) measurements showed several underestimations in a number of regions across Europe. This is a known problem and was already documented in (Bessagnet et al., 2012). The result of the kernel-method over Baden-Württemberg (Manheim – Stuttgart region) is given in in the lower half of Figure 1.

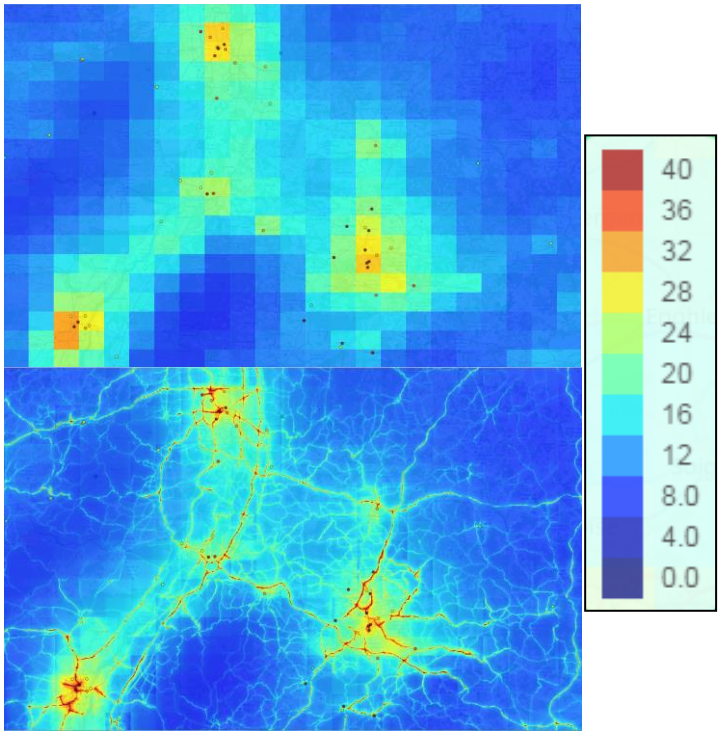

Figure 1: Extracts of the NO_2 maps over Baden-Württemberg (Manheim – Stuttgart). Upper figure depicts the CHIMERE-NO_2 map. Lower figure shows the 125x125m² kernel map. All data are annual mean NO_2-concentrations for the year 2010 with units in µg/m3.

To validate the newly produced NO_2 kernel map, we make use of the AIRBASE monitoring archive. Within the CHIMERE domain, 2,459 yearly average NO_2-measurements are available for the year 2010. This selection excludes locations inside street canyons since the representativeness of these locations is deemed incompatible with the applied methodology.

The results of the validation are presented in Table 1. By applying the kernel method, a clear decrease in BIAS by nearly 10 percentage points is observed (both for the original and the bias corrected CHIMERE results), a slight decrease of RMSE (root mean square error), and a clear increase in spatial correlation between the CHIMERE basemap and the kernel map. The percentage of monitoring stations where the FAIRMODE Modelling Quality Objective (MQO) is met increases from 61 to 68 %, and a decrease in the 90%-percentile Modelling Quality Indicator (MQI) is observed. Note that the MQO of 1 is not met for any of the maps. In general, we can state that the application of the kernel methodology clearly increases the accuracy of the EU-wide NO_2 assessment compared to the CHIMERE regional background maps. It must be noted however that the raw CHIMERE assessment shows a significant underestimation of the observed NO_2 concentrations. This results also in underestimations in the kernel-map.

Table 1 : Validation statistics for the various runs.

	CHIMERE	**CHIMERE + kernel**
BIAS	-28%	-19%
RMSE	56%	50%
BCRMSE	48%	46%
R^2	0.34	0.43
Slope_orthogonal	0.96	1.11
Intercept_orthogonal	-6.15	-7.70

Ratio of standard deviations	0.98	1.07
% stations fulfilling the MQO	61%	68%
MQI	2.14	1.89

Based on comparison with the individual bottom-up maps, kindly provided by several European teams, we can conclude that:

- The main differences between the bottom-up maps and the kernel map is found in the background concentrations.
- Changing of proxies between OTM (Open Transport Map, http://opentransportmap.info/) and a more ad hoc disaggregation of Open Street Maps only give rise to small changes.
- Inclusion of major tunnels in the kernel model is important to reproduce local concentration patterns.
- Some roads, such as the M25 in London, seem to be underestimated in the gridded 7km SHERPA emission dataset.

CONCLUSIONS

In this contribution, we present the development of a modelling approach that can be used to quickly calculate European-wide annual average NO_2-concentration maps, both in assessment and in scenario mode. It was shown that using this kernel methodology improves the performance, as measured for example by bias and RMSE, compared to a 7km resolution model.

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