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Supplement of

Top–down quantification of NO_x emissions from traffic in an urban area using a high-resolution regional atmospheric chemistry model

Friderike Kuik et al.

Correspondence to: Friderike Kuik (friderike.kuik@gmail.com)

S1 Changes to the model code and impact on results

S1.1 Code changes

The WRF-Chem code file dry_dep_driver.F (v.3.8.1) was changed in order to also allow for increased nighttime mixing in grid cells with high emissions in case an urban physics scheme is used (starting from line 685):

```
     if (p_e_co >= param_first_scalar )then
! if (sf_urban_physics .eq. 0 ) then
         if (emis_ant(i,kts,j,p_e_co) .gt. 0) then
          ekmfull(kts:kts+10) = max(ekmfull(kts:kts+10),1.)
         endif
         if (emis_ant(i,kts,j,p_e_co) .gt. 200) then
          ekmfull(kts:kte/2) = max(ekmfull(kts:kte/2),2.)
         endif
         if (p_e_pm25i > param_first_scalar )then
          if (emis_ant(i,kts,j,p_e_pm25i)+ emis_ant(i,kts,j,p_e_pm25j)
           .GT. 8.19e-4*200) then
           ekmfull(kts:kte/2) = max(ekmfull(kts:kte/2),2.)
          endif
         endif
         if (p_e_pm_25 > param_first_scalar )then
          if (emis_ant(i,kts,j,p_e_pm_25) .GT. 8.19e-4*200) then
           ekmfull(kts:kte/2) = max(ekmfull(kts:kte/2),2.)
          endif
! endif
         endif
```

S1.2 Impact of code changes

Two test simulations illustrate the impact of some of the modifications made to this model setup with respect to Kuik et al., 2016. The differences between the two model simulations shown in this section are the application of the above-described modification or not, and the use of default (TNO) diurnal cycles of traffic emissions and a diurnal cycle calculated based on traffic counts in Berlin. The latter is expected to mainly impact the results during daytime for urban background stations and, to a smaller extent, suburban background stations. The figures show results for simulated and observed NO_2 concentrations.

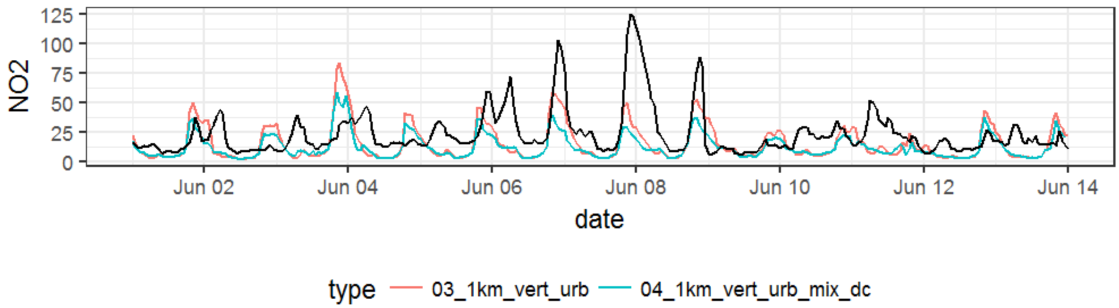

Figure S1. Comparison of modelled NO_2 concentrations of simulations without modified mixing routine and default diurnal cycle of traffic emissions (03_1km_vert_urb) and with modified mixing routine and a diurnal cycle of traffic emissions calculated based on traffic counts in Berlin (04_km_vert_urb_mix_dc). The black line shows observations. Results are averaged over all urban background stations used in this study.

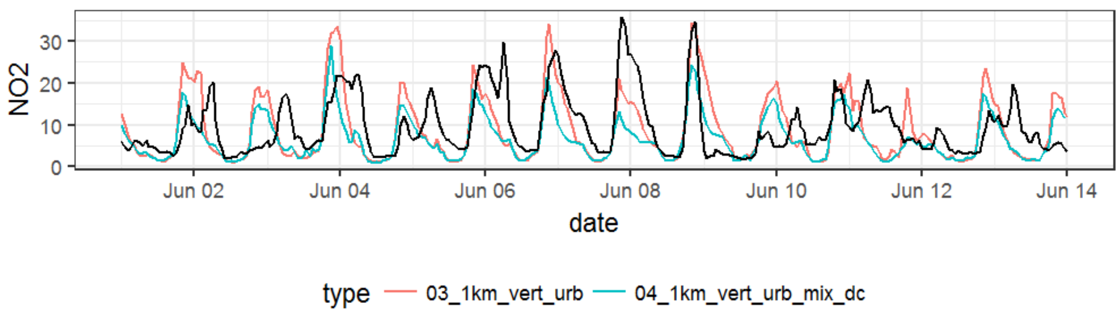

Figure S2. As Fig. S1, but for suburban background stations.

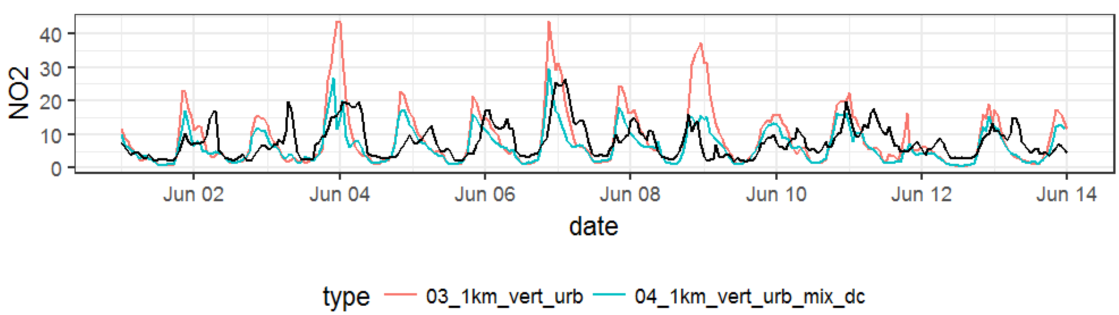

Figure S3. As Fig. S1, but for rural background stations.

S2 Emission processing

S2.1 Downscaling

We used TNO-MACC III emission data and in cooperation with TNO downscaled the data from a horizontal resolution of ca. 7kmx7km to a ca. 1kmx1km. We based the downscaling on proxy data, including population density (Environment Database of the Berlin Senate Department for the Environment, Transport and Climate Protection, Landscan 2010 data), traffic density for the area of Berlin (Environment Database of the Berlin Senate Department for the Environment, Transport and Climate Protection) and the road network of Brandenburg (OpenStreetMap). Population data is used to downscale emissions from residential combustion (SNAP2) and product use (SNAP6), traffic data is used to downscale emissions from traffic (SNAP 71-75). The 1kmx1km emission grid is defined so that each coarse grid cell of 7kmx7km is divided into 7x7 parts. From each of the proxy datasets a factor is then calculated indicating the proportion of each proxy data type in one high resolution grid cell within one coarse grid cell. These factors are used in order to downscale the respective emissions in the respective area.

S2.2 Modification of airport emissions for Berlin

Airport emissions in Berlin, designated by point sources within non-road transport emissions in the TNO-MACC III inventory, are split into airport emissions into emissions on the ground and emissions from the LTO-cycle. We attribute 60% of the emissions to emissions on the ground, and the remaining emissions to emissions from the LTO cycle, where we distribute the emissions equally into all layers below 900m. The LTO-cycle includes emissions from takeoff, landing and aircraft cruise up to ca. 900m. Furthermore, the TNO-MACC III inventory still includes emissions from the Berlin-Tempelhof airport, which has been closed to air traffic in 2008. In addition, emissions from Tegel airport seemed unrealistically larger than emissions from Schönefeld airport. Thus we summed the emissions from all three major airports in the Berlin-Brandenburg region included in the TNO-MACC III inventory and re-distributed them onto the two airports active in 2014, based on activity data, attributing 75% of the emissions to Tegel and 25% to Schönefeld.

S3 Model evaluation

S3.1 Observations

Table S1. Coordinates, names, codes (airbase) and station types of measurement stations used in this paper. Different from what is indicated in the airbase metadata, the station DEBE066 has been defined as suburban background station in this paper, as its characteristics and location are more in line with suburban background conditions in Berlin than with urban background conditions.

Station code	Station name	Station type	Longitude	Latitude
DEBE027	Schichauweg	rural-nearcity background	13.368	52.398
DEBE032	Grunewald	rural-nearcity background	13.225	52.473
DEBE056	Mueggelseedamm	rural-nearcity background	13.647	52.448
DEBE062	Frohnau	rural-nearcity background	13.296	52.653
DEBB075	Gross Glienicke	suburban background	13.124	52.484
DEBB086	Blankenfelde-Mahlow	suburban background	13.424	52.35
DEBE051	Buch	suburban background	13.49	52.644
DEBE066	J. u. W. Brauer Platz	suburban background	13.53	52.485
DEBE010	Amrumer Str.	urban background	13.349	52.543
DEBE018	Belziger Str.	urban background	13.349	52.486
DEBE034	Nansenstr.	urban background	13.431	52.489
DEBE068	Brueckenstr.	urban background	13.419	52.514
DEBE061	Schildhornstr.	urban traffic	13.318	52.464
DEBE063	Silbersteinstr	urban traffic	13.442	52.468
DEBE064	Karl Marx Str.	urban traffic	13.434	52.482
DEBE065	Frankfurter Allee	urban traffic	13.47	52.514
DEBE069	Mariendorfer Damm	urban traffic	13.388	52.438

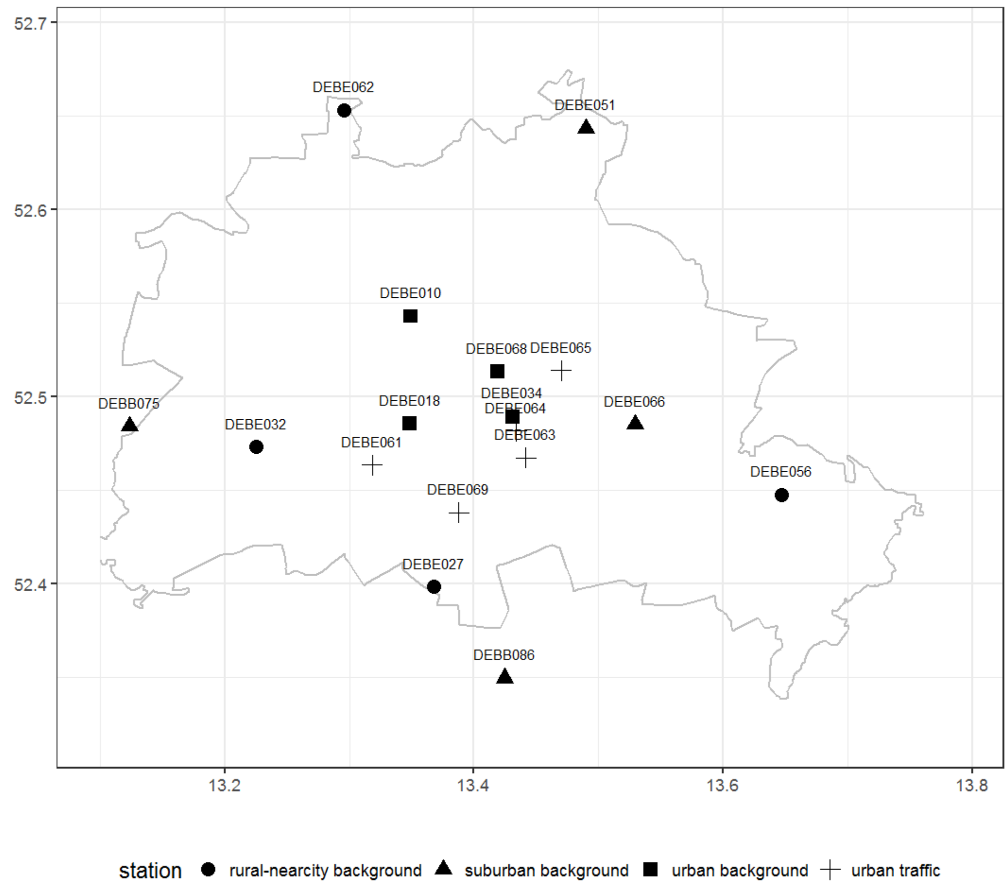

Figure S4. Locations of measurement stations used in this paper including their station type and airbase code.

S3.2 Statistical indicators

The statistical indicators used in this study include the mean bias (MB), normalized mean bias (NMB), root mean square error (RMSE) and Pearson correlation coefficient (R) and are defined as follows, with the model results M, observations O, number of model-observations pairs N and standard deviation σ:

$$MB = \sum_{i=1}^{N}(M_i - O_i) \tag{1}$$

$$NMB = \frac{\sum_{i=1}^{N}(M_i - O_i)}{\sum_{i=1}^{N} O_i} \tag{2}$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)} \tag{3}$$

$$R = \frac{\frac{1}{N}\sum_{i=1}^{N}(M_i - \overline{M})(O_i - \overline{O})}{\sigma_M \sigma_O} \tag{4}$$

S3.3 Additional model performance indicators

In addition to the model quality objective (MQO), performance indicators for the mean bias and normalized mean bias are indicated in the manuscript and defined as follows, following Pernigotti et al. (2013):

$$|NMB| < \frac{2RMS_U}{\overline{O}} \tag{5}$$

$$|MB| < 2U(\overline{O}) \tag{6}$$

With the root mean square of the measurement uncertainty

$$RMS_U = \sqrt{\frac{1}{N}\sum_{i=1}^{N} U_{O_i}^2} \tag{7}$$

and $U(\overline{O})$ the uncertainty of the mean of the observed time series.

S4 Spectral decomposition

Observed and modelled time series are spectrally decomposed into a long term (LT), synoptic (SY), diurnal (DU) and intra-diurnal (ID) component, following Hogrefe et al. (2000), and Galmarini et al. (2013). A Kolmogorov-Zurbenko filter $kz_{m,k}$ was used with the time windows m and smoothing parameter k, time series x and time t:

$$ID(t) = x(t) - kz_{3,3}(x(t)) \tag{8}$$

$$DU(t) = kz_{3,3}(x(t)) - kz_{13,5}(x(t)) \tag{9}$$

$$SY(t) = kz_{13,5}(x(t)) - kz_{103,5}(x(t)) \tag{10}$$

$$LT(t) = kz_{103,5}(x(t)) \tag{11}$$

The decomposition was done in R, using the library *kza*.

S5 Supplementary figures

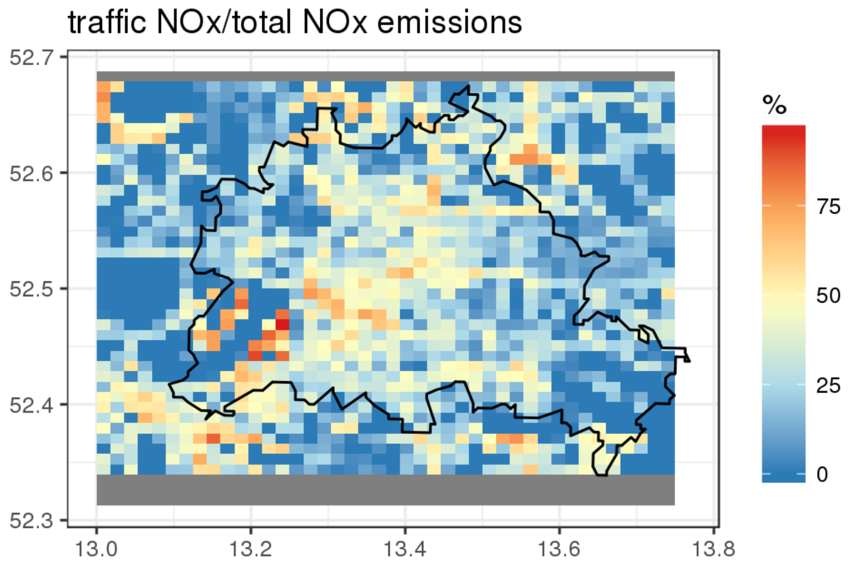

Figure S5. Contribution of traffic NOx emissions to total annual surface NOx emissions in the Berlin-Brandenburg area, based on the downscaled version of TNO-MACC III.

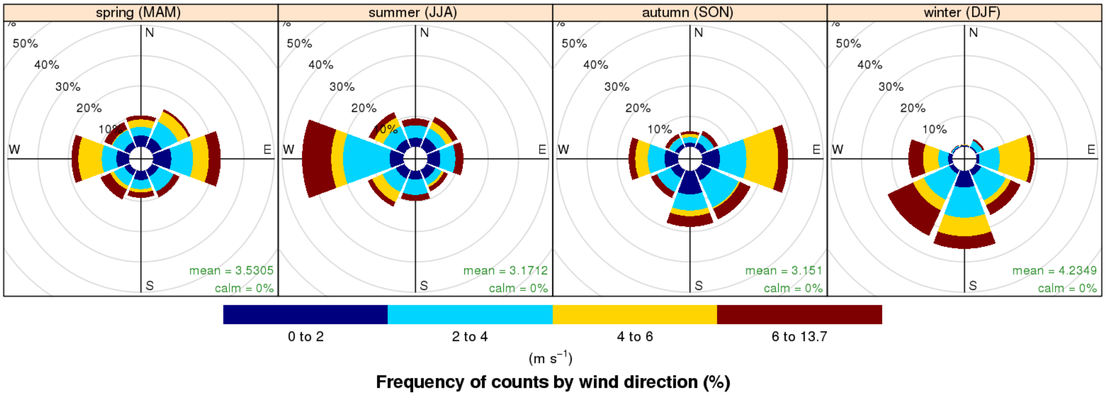

Figure S6. Wind rose showing the frequency distribution of wind speed and direction for the Berlin DWD stations, observations.

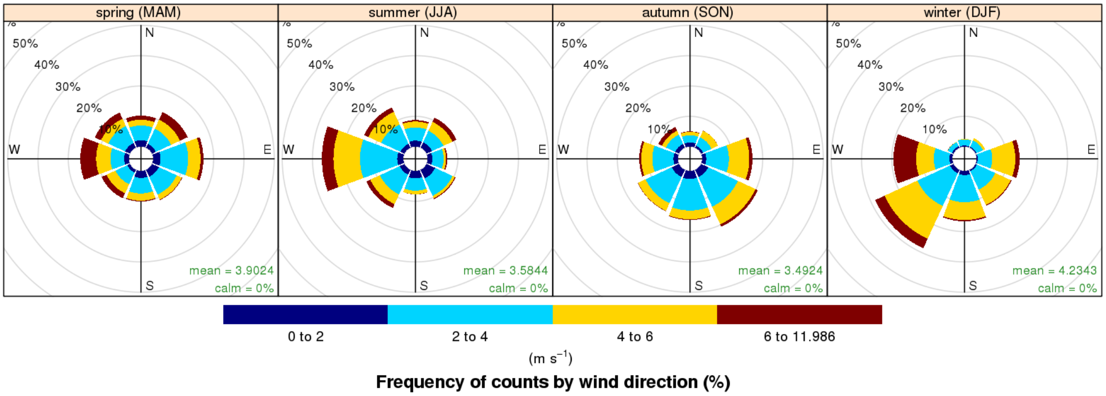

Figure S7. Wind rose showing the frequency distribution of wind speed and direction for the Berlin DWD stations, model results.

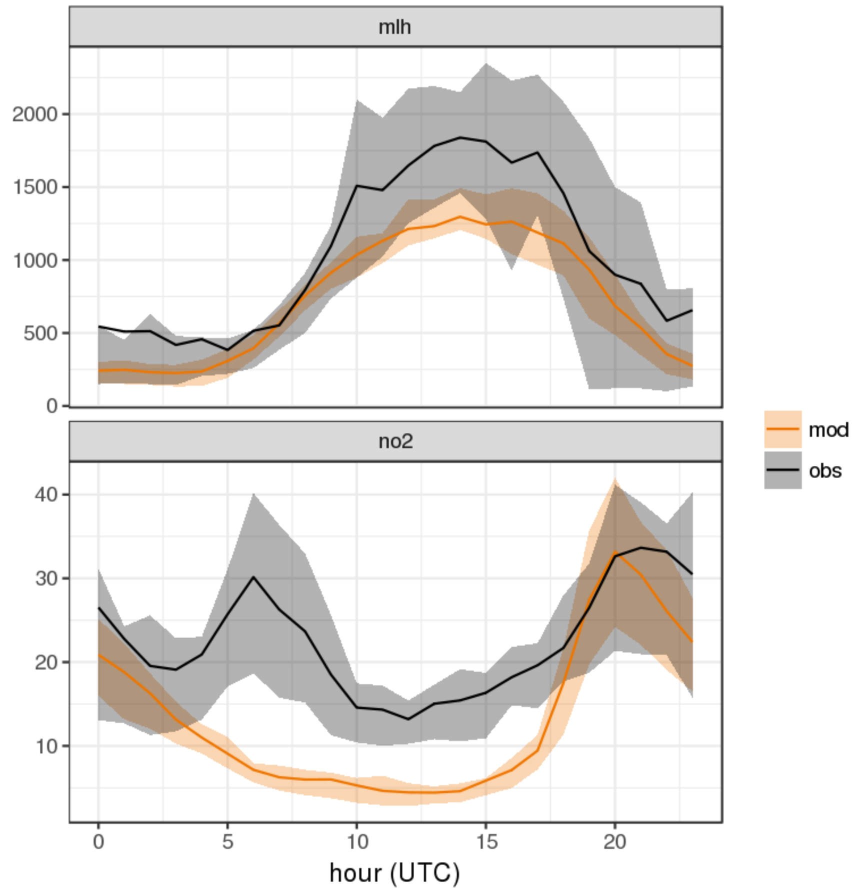

Figure S8. Mean diurnal cycles of observed (obs) and modelled (mod) mixing layer height (MLH) and NO_2 concentrations at Nansenstraße. All data are only averaged over times when MLH observed with a ceilometer is available. This includes between 24-57 hourly values between 20 June and 27 August 2014. The shaded areas show the 25th and 75th percentiles of the data. MLH is given in m, NO_2 concentrations are given in μg m^{-3}.

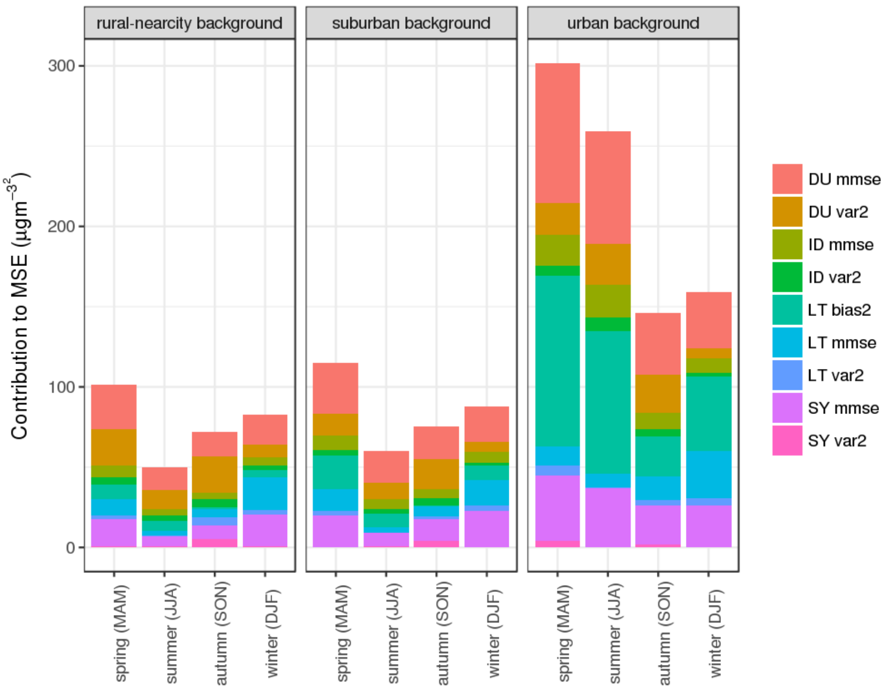

Figure S9. Contribution to mean square error of model results per season and station class.

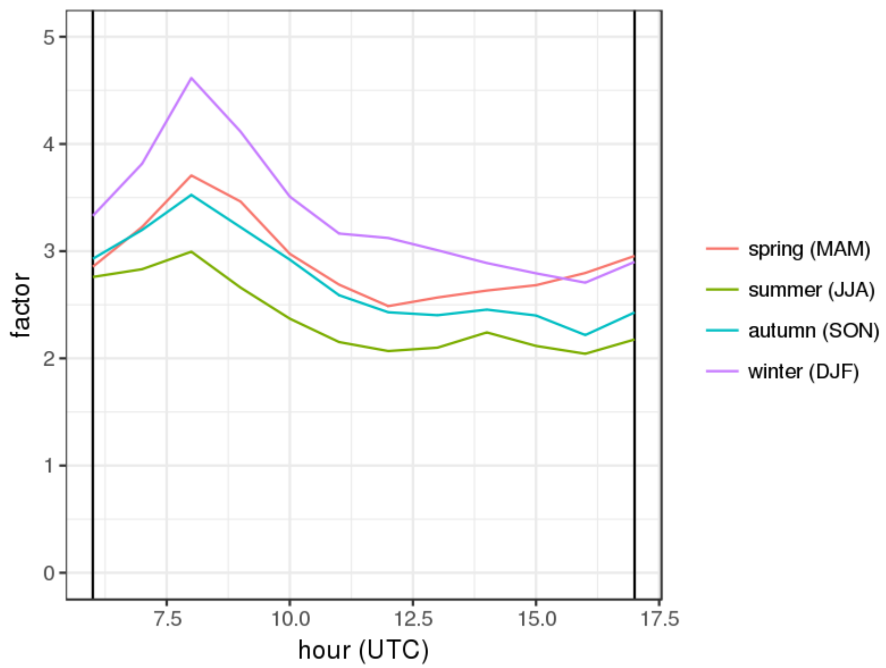

Figure S10. Time- and season-dependent NO_x-emission correction factor.