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Evaluation of a high resolution regional atmospheric chemistry model using MAX-DOAS and in situ NO_2 measurements

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Regional atmospheric chemistry models are adopted for simulating concentrations of atmospheric components at high resolution and quantifying the impact of localized emissions (e.g. industrial and urban clusters) on the non-linear chemical processes, e.g. ozone production. However, their evaluation is challenging due to the limited availability of high spatiotemporally resolved reference datasets. For the same reason, the vertical distribution of pollutants simulated by the model is especially arduous to assess.

Here, we present regional atmospheric chemistry model studies with spatial resolution up to 2.2 × 2.2 km^2 focused around Germany for May 2018 using the MECO(n) model system. Using a network of surface concentration measurements at background, near traffic and industrial locations, we evaluate the spatial distribution of NO_2 simulated by the model. The highly resolved model together with a comparable resolution and up-to-date input emissions inventory, was found to perform best in reproducing the spatial distribution of NO_2 surface volume mixing ratios (VMRs). We propose a computationally efficient approach to account for the diurnal and day of the week variability of input anthropogenic emissions (e.g. from road transport), which proved to be crucial for resolving the temporal variability of NO_2 surface VMRs.

The simulated NO_2 tropospheric vertical column densities were evaluated by employing the measurements of a 4-azimuth MAX-DOAS instrument in Mainz. Generally, such comparisons do not account for the spatial sensitivity volume of the MAX-DOAS measurements, the change of sensitivity within this volume and the spatial heterogeneity of NO_2. We therefore apply a consistent approach of comparison of the differential slant column densities (dSCDs), which overcomes these limitations. Moreover, the dSCDs are obtained for several elevation and azimuth angles, which are characterized by distinctive sensitivity for different vertical levels within the boundary layer and different horizontal representativeness. Hence, also an evaluation of the model in simulating the vertical distribution of NO_2 can be performed with this approach using continuous MAX-DOAS measurements spanning long time periods. We found that the model performs well with respect to the measured dSCDs at low elevation angles (< 8°) with an overall bias between +14 and -9%, and Pearson correlation coefficients between 0.5 and 0.8 for the

different azimuth viewing directions.