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Validation of a regional chemistry model over Germany using 4-azimuth MAX-DOAS measurements and satellite observations

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Satellite observations of atmospheric trace gases like NO_2 often underestimate the traces gases over urban and industrial locations if compared with ground-based MAX-DOAS measurements. This is partially due to the satellite airmass factors being calculated based on model results for rather at coarser spatial resolution ($\sim$ 100 km) than the satellite observation. Concentrations close to the surface are thus systematically underestimated resulting in high biased airmass factors and low biased vertical column densities (VCD). Regional models (e.g. COSMO) can simulate the atmospheric physical and chemical state at a high spatial resolution of less than 10 km. However, regional models themselves need to be validated beforehand.

A 1-way nested MECO(3)1 coupled model system was set-up for Germany, in which the finer resolved domain receives the initial and boundary conditions online from the coarser regional or global model. Simulations at domains over Germany at $\sim$7 km $\times$ 7 km spatial resolution and over Rhineland-Palatinate at $\sim$2.2 km $\times$ 2.2 km spatial resolution were performed simultaneously for March - April 2018. Deep convection is resolved in the finest domain whereas shallow convection is parametrised based on the so-called Tiedtke scheme. We have used the TNO MACC III emission inventory and MIME mechanism for chemical calculations within the model system. Meteorological evaluation against ECMWF reanalysis dataset was carried out to optimize the model dynamics, and the optimum simulation duration after which a restart of meteorological calculation was required.

The 3-D fields HCHO and NO_2 derived from the model are evaluated against the corresponding slant column densities (SCDs) measured by a 4-Azimuth MAX-DOAS instrument operational at the rooftop of our institute in Mainz. For that purpose height-resolved 2-D box airmass factors were calculated using the McArtim (Monte Carlo Atmospheric radiative transfer model) and applied to the modelled trace gas profiles along elevation angles of the measurements for the study period. This comparison procedure accounts for the complex dependency of the MAX-DOAS SCDs on the 3D (vertical and horizontal) trace gas distribution in the measurement direction.

NO_2 tropospheric vertical column densities are also calculated for the domain with coarser spatial resolution (7 km $\times$ 7 km) simulations. Simulated tropospheric VCDs are validated against TROPOMI observations. For the intercomparison, we have modified the airmass factors in the TROPOMI data product using the model calculated NO_2 a priori profile and taking into account averaging kernels and tropopauses level. This resulted in a better agreement of the spatial pattern of NO_2 VCDs between model and satellite.