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NitroNet – A new deep-learning model for the prediction of NO₂ profiles based on TROPOMI satellite observations

Leon Kuhn^{1,2}, Steffen Beirle¹, and Thomas Wagner^{1,2} ¹Max Planck Institute for Chemistry, Satellite Group, Mainz, Germany (l.kuhn@mpic.de) ²Institute for Environmental Physics, University of Heidelberg, Heidelberg, Germany

Nitrogen dioxide (NO₂) is an important air pollutant and has been widely recognized for its hazardous impact on human health. Tropospheric NO₂ is routinely monitored using satellites (e.g. TROPOMI onboard Sentinel-5P), in situ instruments, and ground-based spectroscopic measurements (e.g. multi-axis differential optical absorption spectroscopy, MAX-DOAS). However, these measurements do not give the full picture: Satellite instruments can only measure the integrated load (column density), in situ measurements are mostly deployed at the surface, and MAX-DOAS instruments are still very sparse. In consequence, it is currently impossible to obtain sufficiently resolved NO₂ profiles from measurements alone. Regional chemistry and transport (RCT) simulations can be used to simulate NO₂ profiles where no observations are available, but they are computationally expensive and require meticulous parameter calibration to achieve acceptable agreement with observational reference data.

We present **NitroNet**, a new deep-learning model for the prediction of tropospheric NO₂ profiles. The model is based on a feedforward neural network, which was trained on a synthetic dataset from the RCT model WRF-Chem. NitroNet receives vertical NO₂ column densities (VCDs) from TROPOMI and ancillary variables (meteorological, emissions, etc.) as input, from which it predicts tropospheric NO₂ concentration profiles. The NO₂ VCD is descriptive of the profiles' magnitudes, while their shapes are derived from the ancillaries (e.g. the boundary layer height). The ancillaries are taken from the TROPOMI NO₂ data product, ERA5 reanalysis data, and the EDGARv5 emission inventory. By prior filtering of the training data based on their agreement to reference data, NitroNet can achieve better agreement with TROPOMI's NO₂ VCDs and surface in situ measurements than WRF-Chem at a much faster runtime. On the downside, these predictions are available only once per day, when the TROPOMI overpass occurs. We showcase the model's performance against a variety of validation data (satellite, in situ, and MAX-DOAS measurements), and its ability to generalize to different seasons and geographical regions.

What makes NitroNet unique in the field of deep-learning air pollution models is its training on *synthetic* data. This conceptual difference to the many recently developed models, trained on empirical observations alone, unlocks important new possibilities: Due to the paucity of other observations, empirical training sets are practically confined to surface concentrations from in situ measurements. Synthetic data generation, on the other hand, allows for training sets with full NO₂

profiles instead. Moreover, synthetic training examples do not suffer from the cross-sensitivities of in situ measurements to other nitrogen compounds (up to a factor of 2).

The NO₂ profiles produced by NitroNet can be used as high-resolution replacements for the a priori profiles in satellite retrievals, or for studies on surface level air pollution.