Supplement: A light-weight NO_2-to-NO_x conversion model for quantifying NO_x emissions of point sources from NO_2 satellite observations

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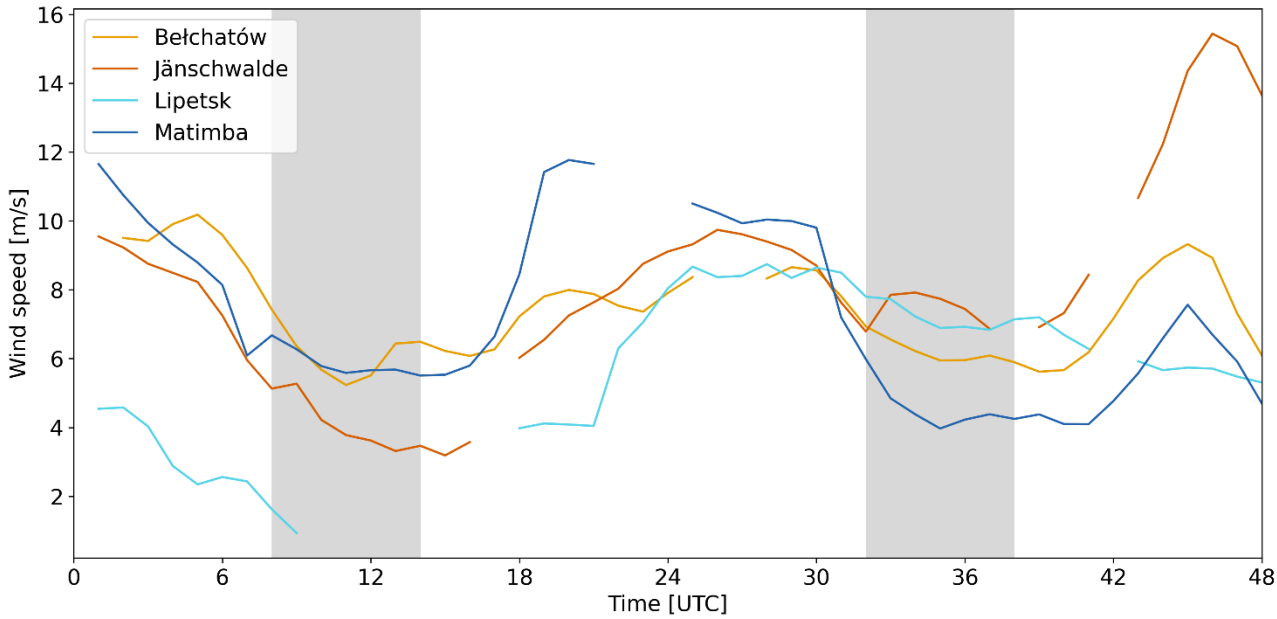

Figure S1: Temporal evolution of vertically weighted wind speeds in the MicroHH simulations of Bełchatów, Jänschwalde, Lipetsk, and Matimba as a function of simulated time steps. Grey shading represents the time steps used in the analysis.

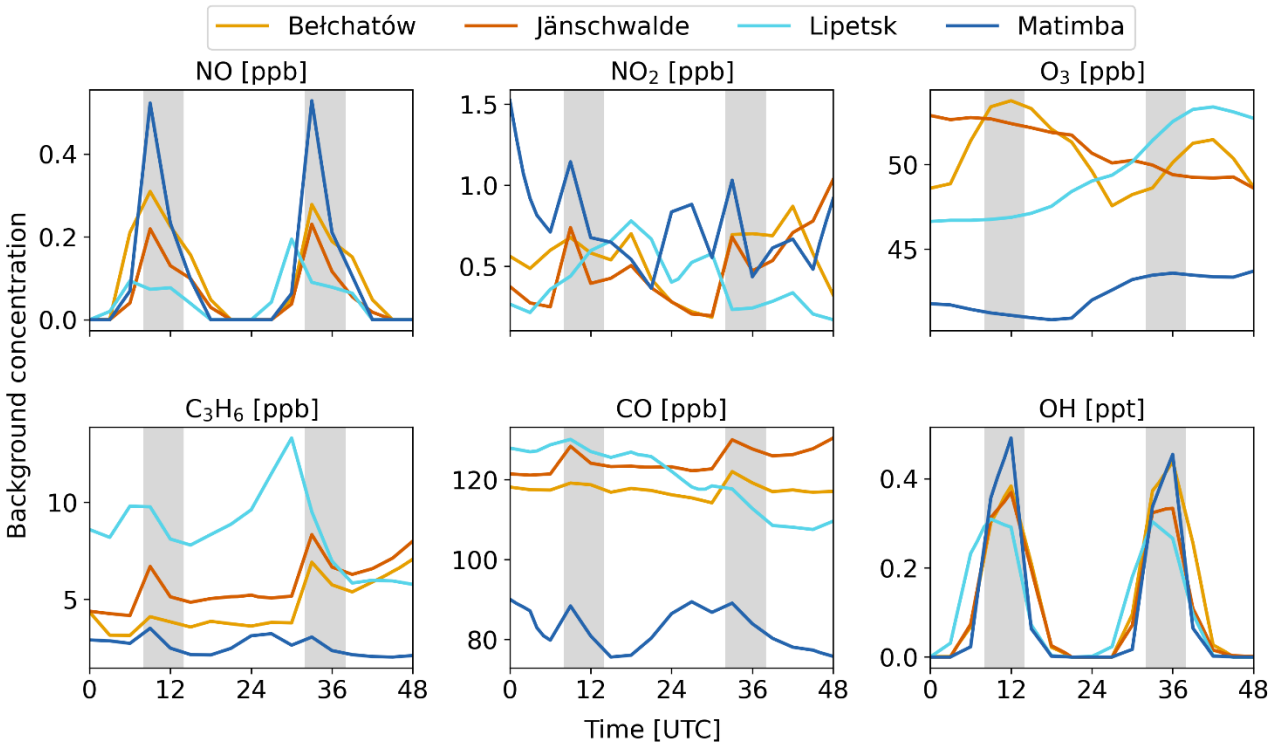

Figure S2: Temporal evolution of mean background concentration of reactive trace gases in the lowest kilometer for the MicroHH simulations of Bełchatów, Jänschwalde, Lipetsk, and Matimba. Grey shading represents the time steps used in the analysis.

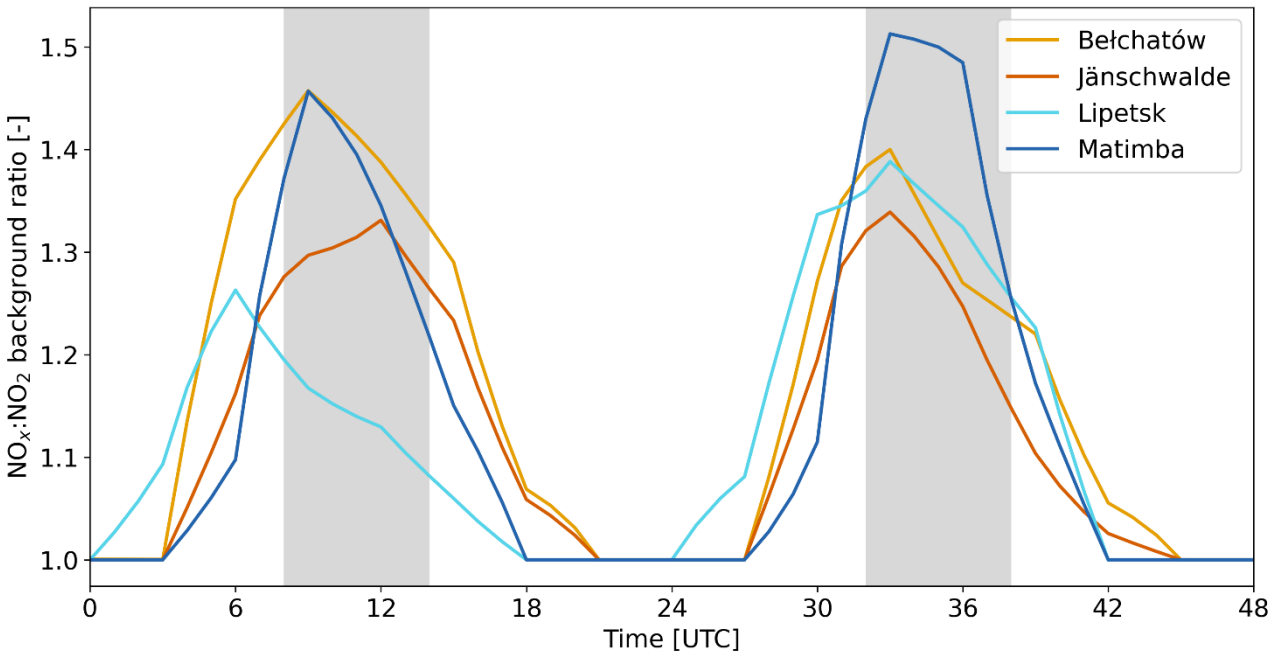

Figure S3: NO_x:NO_2 ratios based on background NO and NO_2 concentrations from CAMS (details in Krol et al. 2024). Grey shading represents the time steps used in the analysis.

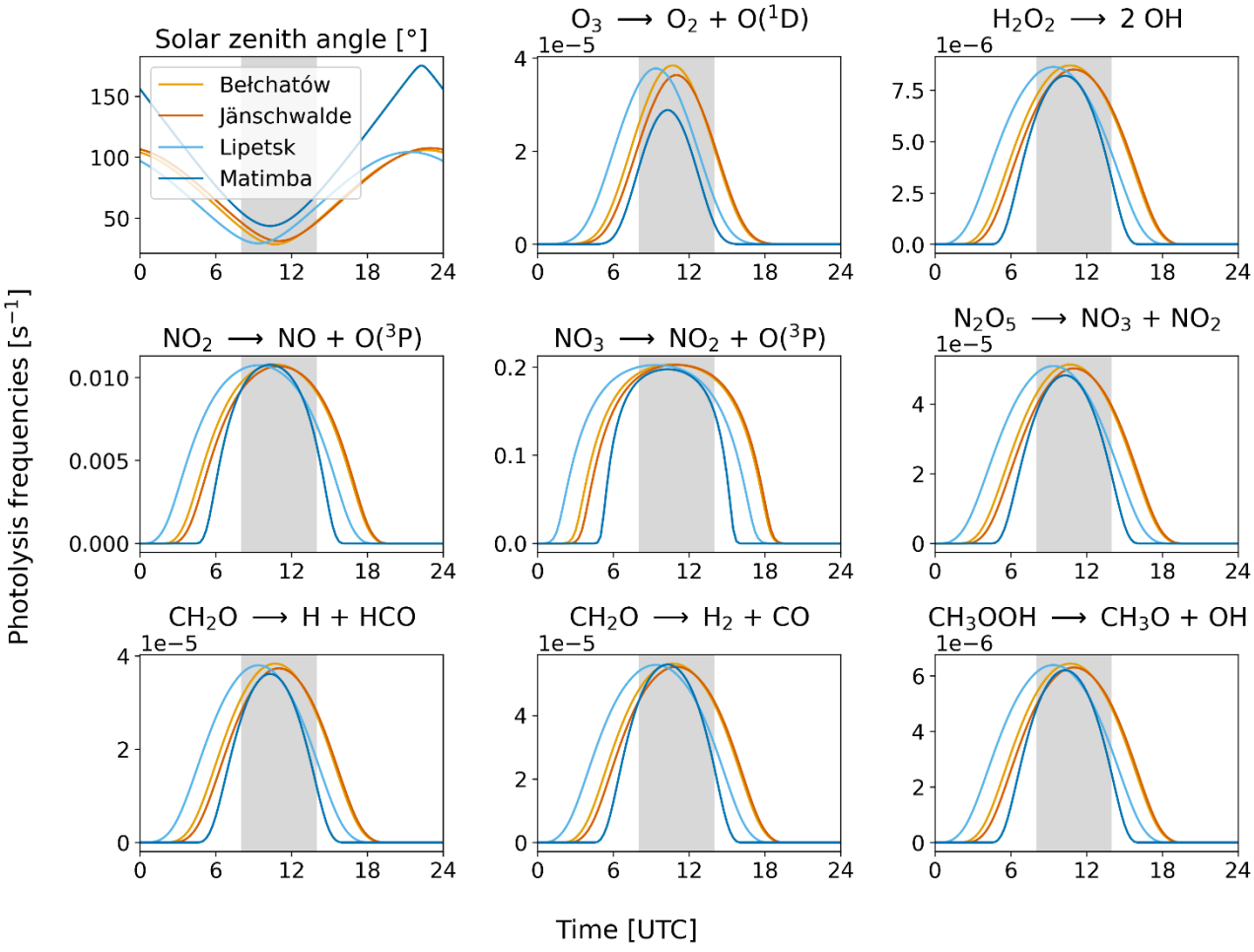

Figure S4: Temporal evolution of solar zenith angle and frequencies of simulated photolysis processes in the MicroHH simulations of Bełchatów, Jänschwalde, Lipetsk, and Matimba. Grey shading represents the time steps used in the analysis.

To study the bias introduced by the assumption of constant NO_2 profiles within the PBL for the re-calculation of AMFs, we have calculated the expected SCDs for the MicroHH simulation of Matimba on the 24th of July 2020 according to Eskes et al. 2022. The SCDs were then converted to VCDs using the updated AMFs which were calculated under the assumption of a constant NO_2 profile of $5 \cdot 10^{-9}$ mol/mol within the PBL. From the resulting data, we estimated the NO_x emissions and compared them to the estimated emissions using the true MicroHH VCDs.

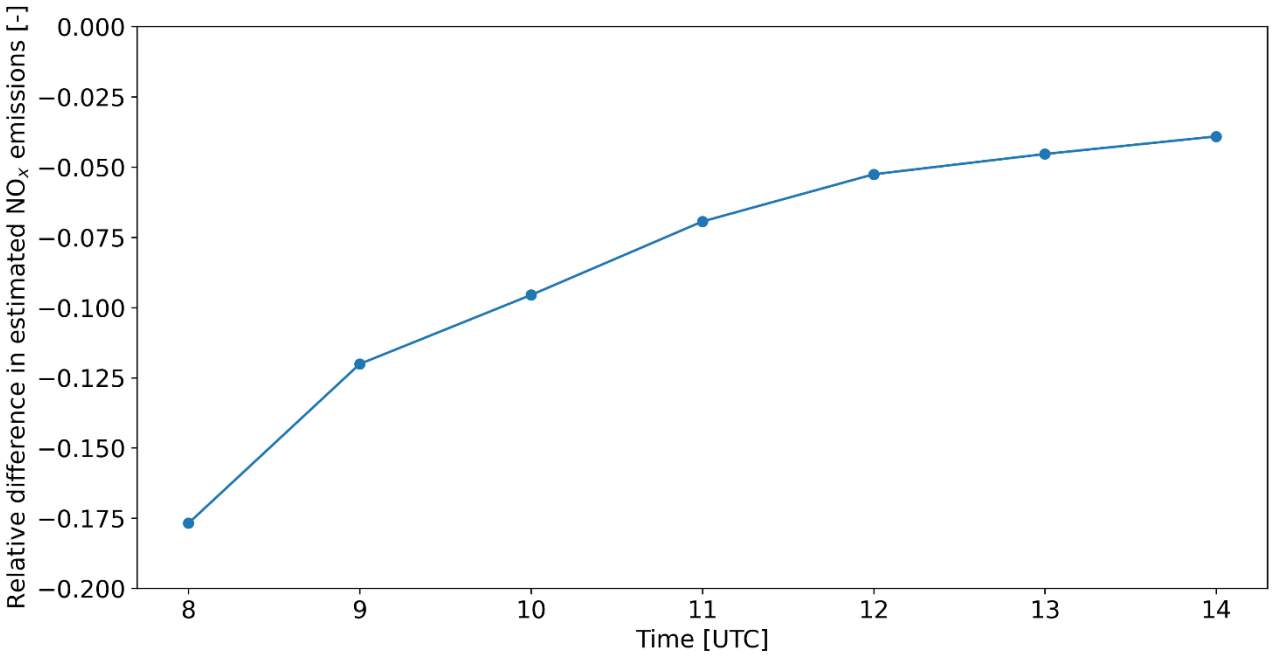

Figure S5: Relative difference in estimated NO_x emissions when re-calculating MicroHH VCDs using the updated AMFs where the NO_2 mole fraction was set to $\mathbf{5 \cdot 10^{-9}}$ mol/mol within the PBL of the detected plumes and estimated NO_x emissions when using the true simulated VCDs in MicroHH.

References

Eskes, H., Van Geffen, J., Boersma, F., Eichmann, K.-U., Apituley, A., Pedergnana, M., Sneep, M., Veefkind, J.P., Loyola, D., 2022. Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Nitrogendioxide.
Krol, M., van Stratum, B., Anglou, I., and Boersma, K. F.: Estimating NOx emissions of stack plumes using a high-resolution atmospheric chemistry model and satellite-derived NO2 columns, https://doi.org/10.5194/egusphere-2023-2519, manuscript in preparation, 2024.