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An improved Bayesian inversion to estimate daily NO_x emissions of Paris from TROPOMI NO_2 observations between 2018–2023

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S1: MicroHH setup

To simulate the NO_2 plume over of a city, we use a simplified version of the MicroHH model that was previously used in Krol et al. (2024). First, instead of using initial chemical and meteorological conditions from the ERA5 and CAMS systems, we use standard profiles to initialise the model (Table S1 and Figure S1).

Table S1: Initial conditions for chemical species and meteorology used to start MicroHH simulations over Paris.

Species	**Mole fraction (nmol/mol)**
CO	90
H_2O_2	1.0
HNO_3	1.0
HCHO	1.0
ROOH	1.0
NO_2	0.1
NO	0.05
Meteorology	**Value (m/s)**
u	5
v	0

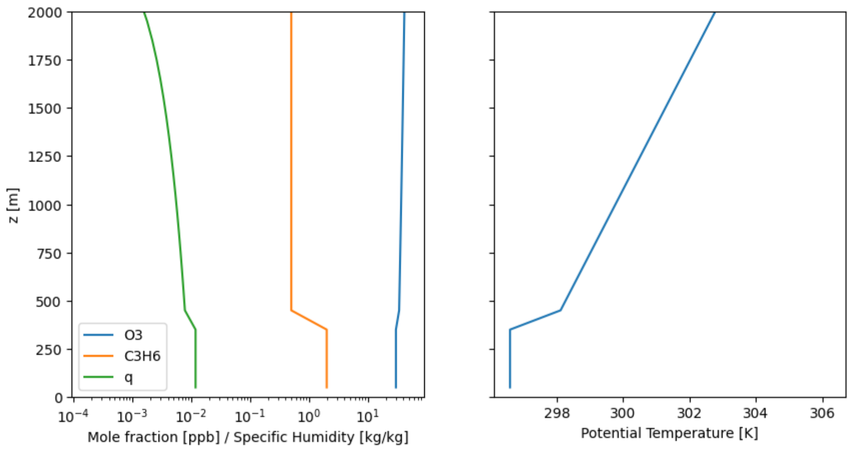

Figure S1: Initial profiles for (left) O_3, C_3H_6 (general hydrocarbon, see Krol et al., 2024), humidity *q*, and (right) potential temperature.

For meteorological variables, we use circular boundary conditions, while for the chemical species we have free outflow at the eastern edge of the domain.

At the surface, we apply a sinusoidal varying forcing for heat and moisture. The maximum heat and moisture fluxes (after 6 hours of simulation) are 0.1 K m/s and 0.15 g/kg m/s, respectively.

For chemical compounds, we emit NO, CO, and C_3H_6 with a Gaussian shape pattern representing a city.

Using the using the Tropospheric Ultraviolet and Visible (TUV) model (Madronich and Flocke, 1999), lookup tables of photolysis rates with a 15-minute time resolution are calculated for conditions encountered in Riyadh. These photolysis rates drive the chemistry in MicroHH.

S2: CAMS-REG v7

CAMS-REGv7 is an updated and improved version of the v4 dataset described by Kuenen et al. (2022). We use this inventory to compare our result with (partly) independent emission information. It is only partly independent because TNO-MACC and CAMS-REGv7 are both based on national reporting and the scaling for TNO-MACC relies on the same country reporting that goes into CAMS-REGv7. We calculated one base NO_x emission value over our Paris domain from the CAMS-REGv7 inventory for 2021, by aggregating the 0.05ºx0.1º (lat-lon) cells within the domain. We then scaled this value by emission totals of France between 2018-2023 to obtain a base value for the other years. We then further scaled these base values, using monthly, daily and hourly emission factors for France for different GNFR sectors using scaling factors from Guevara et al. (2020). For 2020 (Covid), 366 separate daily scaling factors are available, which we used for this year.

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