Supplement

Table S1: List of meteorological and air quality measuring stations utilized for comparison.

Site name	Latitude, °N	Longitude, °E	Measured quantity (units)
METEOROLOGY			
STABROEK	51.3493	4.3789	Temperature (°C), Total precipitation (mm), Wind speed (m/s) Wind direction (°)
SINT-KATELIJNE-WAVER	51.0696	4.5346	Min and max humidity (%) Pressure (hPa) Solar irradiance (Wh/m^2)
DIEPENBEEK	50.9155	5.4503	Mixing layer height (m)
UCCLE	50.7975	4.3594	Mixing layer height (m), Ozone mixing ratio (ppm) Pressure (hPa) Temperature (K) Relative humidity (%) Wind speed (m/s) Wind direction (°)
AIR QUALITY			
MARIAKERKE	51.0670	3.6828	NO, NO$_2$
OOSTEEKLO	51.190	3.6873	NO, NO$_2$
WONDELGEM	51.0890	3.7161	NO, NO$_2$
GENT	51.0583	3.7293	NO, NO$_2$, O$_3$, CO
EVERGEM	51.1247	3.7395	NO, NO$_2$
GENT (G.Carlierlaan)	51.0407	3.7350	NO, NO$_2$

DESTELBERGEN	51.0613	3.7753	NO, NO_2, O_3
SINT-KRUIS-WI	51.1501	3.8087	NO, NO_2, O_3
ZELZATE	51.1961	3.8229	NO, NO_2
WACHTEBEKE	51.1761	3.8699	NO, NO_2
DOEL	51.3182	4.2626	NO, NO_2
KALLO	51.2630	4.2789	NO, NO_2
ANTWERPEN	51.25010	4.3421	NO, NO_2
ANTWERPEN	51.2643	4.3413	NO, NO_2
BERENDRECHT	51.3488	4.3397	NO, NO_2, O_3
STABROEK	51.3277	4.3623	NO_2
ANTWERPEN	51.2814	4.3858	NO, NO_2
ANTWERPEN	51.2558	4.3854	NO, NO_2
ANTWERPEN (Groenenborgerlaan)	51.1771	4.4179	NO, NO_2
ANTWERPEN (Belg)	51.2082	4.4216	NO, NO_2
ANTWERPEN	51.2610	4.4244	NO, NO_2
ANTWERPEN (Park Spoor Noord)	51.2286	4.4285	NO, NO_2
BORGERHOUT	51.2097	4.4318	NO, NO_2, O_3, CO
KAPELLEN	51.3204	4.4448	NO, NO_2
SCHOTEN	51.2521	4.4914	NO, NO_2, O_3
AARSCHOT	50.9775	4.8376	NO, NO_2, O_3
LAAKDAL	51.1204	5.02155	NO, NO_2

Table S2: Statistics of model comparisons (correlation coefficient, root mean square error and mean bias) against meteorological data for the PBL sensitivity simulations described in Section 4.1 (Table 3). Statistics are obtained for the ensemble of measurement sites detailed in Table S1. The values shown in red highlight the three worst performing parameterization schemes for each statistic and variable.

CEILOMETER			
Mixing Layer Height			
	R^2	Root mean squared error	Mean bias
P1	0.687	309	-208.1
P2	0.688	264	-102.1
P4	0.504	413	225.8
P5	0.767	245	-166.6
P6	0.789	262	-202.0
P8	0.657	325	-205.2
P9	0.586	385	-295.0
P10	0.416	339	148.3
P11	0.682	313	-220.9
P12	0.606	403	-322.2
SURFACE			
Temperature			
P1	0.984	1.142	-0.144
P2	0.982	1.275	-0.371
P4	0.986	1.391	-0.867
P5	0.98	1.281	-0.45
P6	0.968	1.937	-1.318
P8	0.981	1.25	0.285
P9	0.981	1.191	0.005
P10	0.95	2.36	0.276
P11	0.984	1.157	-0.279
P12	0.982	1.147	-0.131
Relative Humidity			
	R^2	Root mean squared error	Mean bias
P1	0.976	5.679	-3.248
P2	0.964	5.793	2.316
P4	0.937	6.548	2.47
P5	0.972	5.026	-2.023
P6	0.966	7.791	5.903

P8	0.969	5.7	-3.259
P9	0.97	6.908	-4.422
P10	0.949	7.796	2.693
P11	0.976	4.986	-2.174
P12	0.976	5.735	-3.679

Solar Irradiance

	R^2	Root mean squared error	Mean bias
P1	0.999	27.208	19.026
P2	0.999	27.245	19.036
P4	0.999	26.829	17.032
P5	0.998	25.071	9.888
P6	0.996	29.843	4.48
P8	0.999	27.275	19.1
P9	0.999	27.022	18.85
P10	0.999	26.745	17.906
P11	0.999	27.291	19.09
P12	0.999	27.188	19.001

Wind Speed

	R^2	Root mean squared error	Mean bias
P1	0.699	1.342	1.14
P2	0.812	1.79	1.642
P4	0.773	1.722	1.479
P5	0.744	1.305	1.142
P6	0.785	1.198	1.023
P8	0.679	1.436	1.182
P9	0.719	1.313	1.112
P10	0.656	1.16	0.92
P11	0.691	1.332	1.128
P12	0.705	1.365	1.164

Wind Direction

	R^2	Root mean squared error	Mean bias
P1	0.852	22.501	13.944
P2	0.884	20.313	13.11
P4	0.601	19.419	11.853
P5	0.876	23.504	17.013
P6	0.89	23.025	17.244

P8	0.859	22.281	15.139
P9	0.865	21.957	14.162
P10	0.785	23.196	8.583
P11	0.85	22.797	14.301
P12	0.859	22.036	13.991

SONDE

Temperature

	R^2	Root mean squared error	Mean bias
P1	0.893	1.028	0.137
P2	0.923	0.749	0.127
P4	0.936	0.726	0.036
P5	0.927	0.791	-0.004
P6	0.925	0.858	-0.576
P8	0.887	1.163	0.548
P9	0.898	1.011	0.094
P10	0.881	1.244	0.407
P11	0.928	0.821	0.143
P12	0.917	0.887	0.143

Relative Humidity

	R^2	Root mean squared error	Mean bias
P1	0.827	7.415	-0.230
P2	0.906	5.856	-0.330
P4	0.833	7.218	0.644
P5	0.839	7.138	-0.023
P6	0.894	7.008	2.53
P8	0.826	7.298	-0.245
P9	0.765	8.387	0.310
P10	0.799	8.329	0.994
P11	0.841	7.035	-0.094
P12	0.8	7.775	-0.094

Wind Speed

	R^2	Root mean squared error	Mean bias
P1	0.491	0.974	0.23
P2	0.34	1.105	0.175
P4	0.354	1.146	0.275

P5	0.569	0.923	0.215
P6	0.477	0.998	0.345
P8	0.645	0.848	0.265
P9	0.596	0.87	0.142
P10	0.524	1.023	0.385
P11	0.44	1.004	0.215
P12	0.565	0.888	0.215

Wind Direction

	R^2	Root mean squared error	Mean bias
P1	0.614	9.838	3.61
P2	0.498	12.925	4.78
P4	0.605	13.162	5.67
P5	0.667	8.945	1.58
P6	0.676	9.06	3.28
P8	0.603	9.33	1.74
P9	0.571	9.462	1.57
P10	0.658	8.975	2.9
P11	0.66	9.053	3.21
P12	0.588	9.453	3.21

Ozone VMR

	R^2	Root mean squared error	Mean bias
P1	0.951	0.003	3.04e-4
P2	0.855	0.005	-2.16e-3
P4	0.967	0.004	-1.32e-3
P5	0.958	0.002	2.09e-4
P6	0.973	0.002	-1.38e-4
P8	0.951	0.003	9.00e-4
P9	0.944	0.003	8.71e-4
P10	0.354	0.007	-3.76e-3
P11	0.951	0.003	3.8e-4
P12	0.957	0.004	3.8e-4

10   **Table S3: Same as Table S2, but for comparisons against NO₂ surface data, as described in Section 4.2.1.**

	R^2	Root mean squared error	Mean bias
P1	0.729	6.011	0.853

P2	0.732	9.353	4.432
P4	0.527	22.578	18.9
P5	0.755	5.635	0.073
P6	0.723	6.338	1.703
P8	0.871	3.71	-0.423
P9	0.737	6.436	0.244
P10	0.455	23.574	20.024
P11	0.716	6.172	0.951
P12	0.798	6.577	1.196
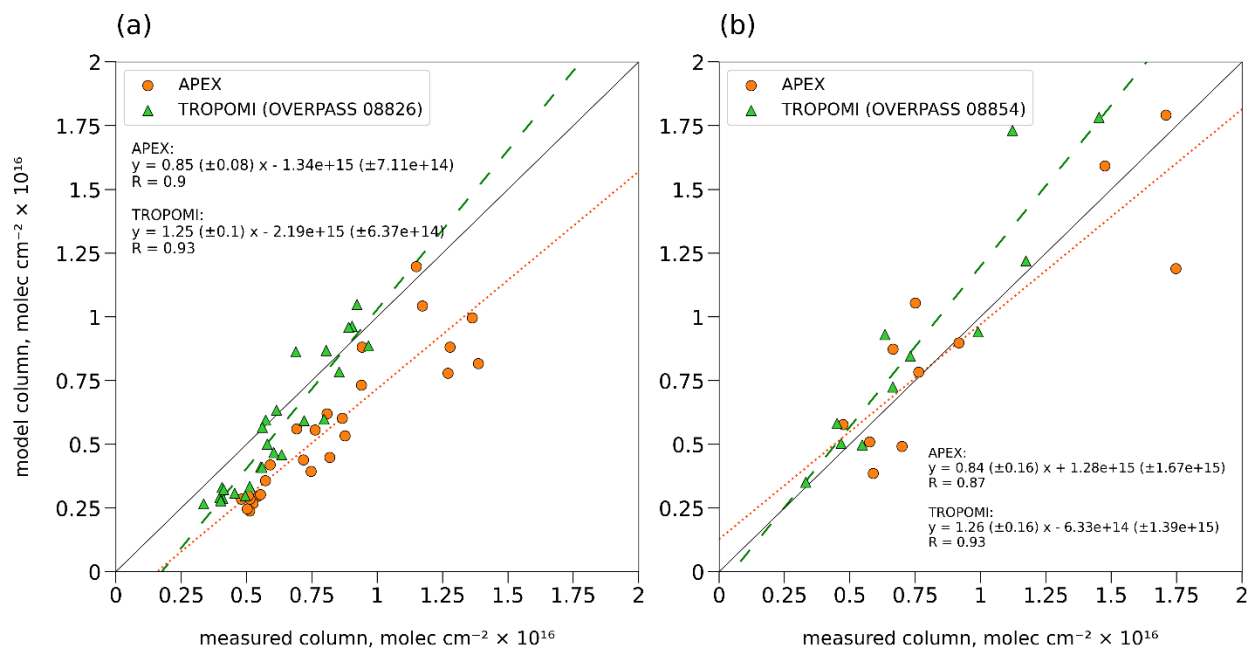
Figure S1. Scatter plots and linear regressions of modelled vs measured columns (APEX and TROPOMI_v1.3) without application of TROPOMI and APEX averaging kernels on model output, on (a) 27th of June and (b) 29th of June. Orange dots and dotted regression lines are for APEX, green triangles and lines for TROPOMI.

15
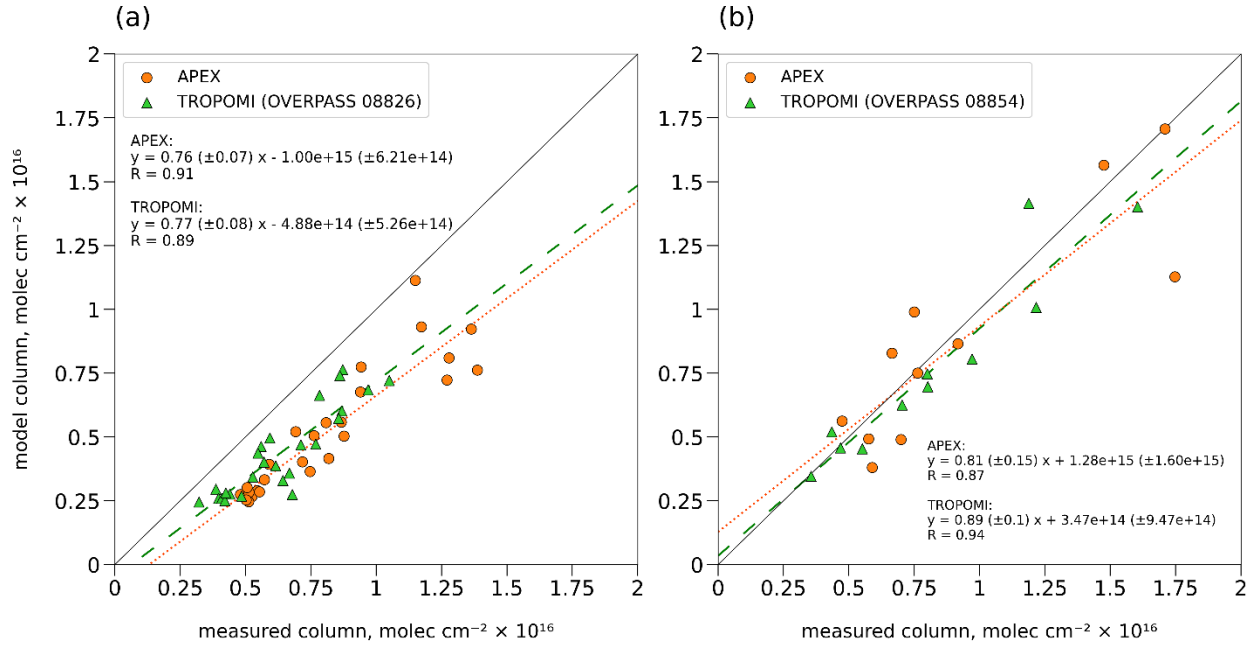
Figure S2. Same as Fig.19, using TROPOMI_PAL.
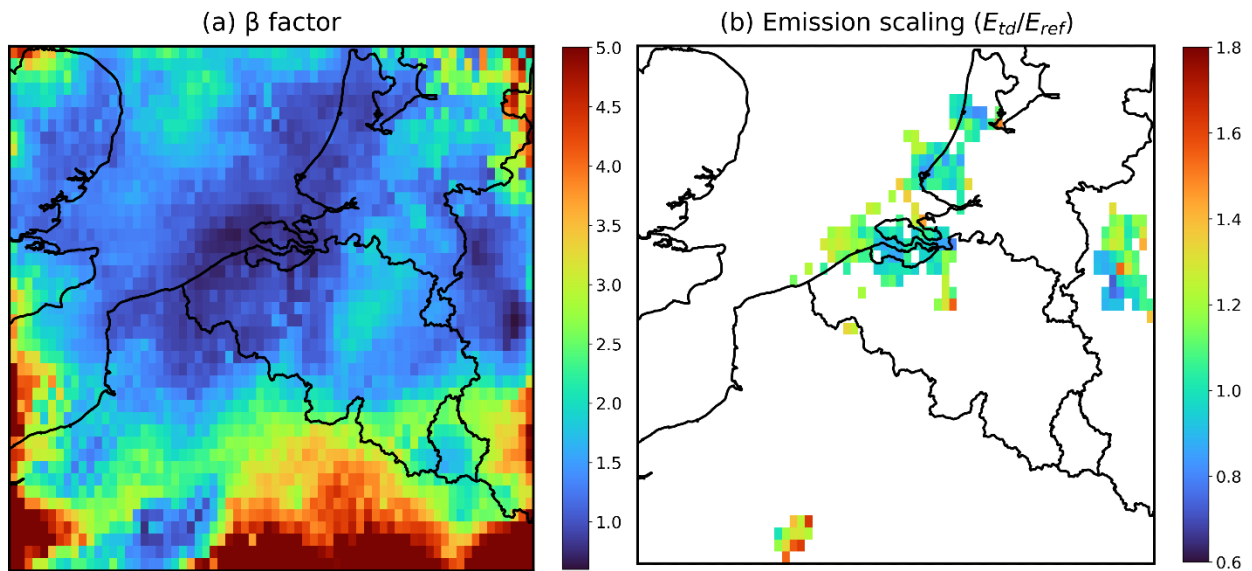
Figure S3. Calculated (a) β factor and (b) emission scaling factor derived from Eq. 4 in order to improve model agreement with bias-corrected TROPOMI data. White pixels indicate pixels removed due to TROPOMI values being too low (<4x10¹⁵ cm⁻²), or β being too high (>1.45). See Section 4.3.3 for details.
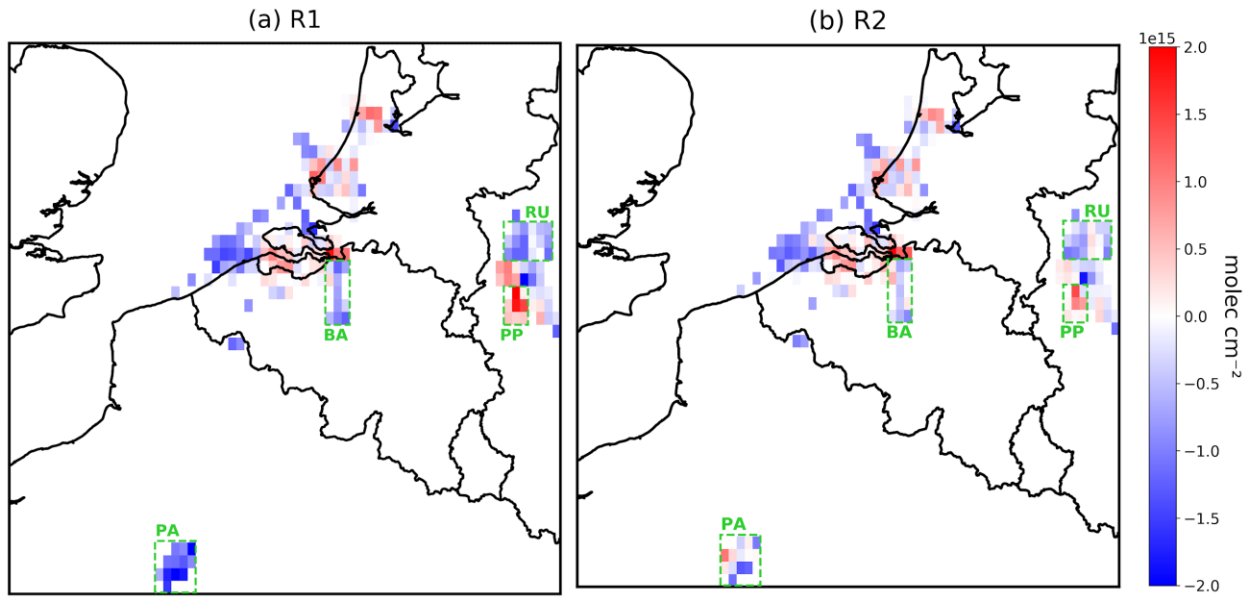
Figure S4. Difference between 15-day averaged WRF-Chem and bias-corrected TROPOMI NO₂, shown for (a) simulation R1, and (b) simulation R2 using top-down emissions. The dashed green boxes represent four regions of interest: Paris (PA), Brussels-Antwerp (BA), the Ruhr area (RU) and a cluster of power plants in Western Germany (PP). Blank areas are pixels for which the emission adjustment is not considered reliable (see text).

25